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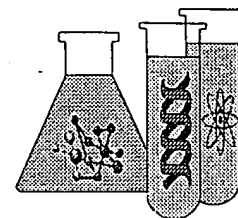
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Technical Info. Specialist
CM1 12014 Tel: 308-4291

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Toby Port
Technical Info. Specialist
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Wei, Y. / au
Mayhew, E

Ahmad, I
Janoff, A

16. A compound having the formula $R^1-Y^1-CHZ^1-CH(NY^2Y^3)-CH_2-Z^2$, wherein:

R^1 is a straight-chained alkyl, alkenyl or alkynyl group having from 5 to 19 carbon atoms in the aliphatic chain;

Y^1 is $-CH=CH-$, $-C\equiv C-$ or $-CH(OH)CH(OH)-$;

Z^1 is OH or a phosphorylcholine attachment-inhibiting group selected from the group consisting of $-X^1$, $-OX^1$, $-X^2X^3$ and $-OX^2X^3$;

Y^2 is H, a phenyl group, an alkyl-substituted phenyl group having from 1 to about 6 carbons in the alkyl chain, or an alkyl chain having from 1 to 10 carbons;

Y^3 is H or a group having the formula $-C(O)R^2$ or $-S(O)_2R^2$;

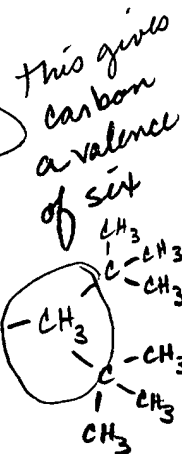
R^2 is a straight-chained alkyl moiety selected from the group consisting of $-(CH_2)_3CH_3$, $-(CH_2)_5CH_3$, $-(CH_2)_7CH_3$ and $-(CH_2)_9CH_3$, an alkenyl group having from 1 to 23 carbon atoms in the aliphatic chain and an alkynyl group having from 1 to 23 carbon atoms in the aliphatic chain;

Z^2 is OH or a phosphorylcholine attachment-inhibiting group selected from the group consisting of $-X^1$, $-OX^1$, $-X^2X^3$ and $-OX^2X^3$;

X^1 is selected from the group consisting of $-C(O)H$, $-CO_2H$, $CH_3(C(CH_3)_3)_2$, $Si(C(CH_3)_3)_3$, $Si(PO_4)_2C(CH_3)_3$, a phenyl group, an alkyl-substituted phenyl group having from 1 to 6 carbons in the alkyl chain, an alkyl chain having from 1 to 6 carbons, an amino group, a fluorine, a chlorine, and a group having the formula $C(R^3R^4)OH$;

X^2 is selected from the group consisting of CH_2- , $C(CH_3)_2-$, $Si(PO_4)_2-$, $Si(CH_3)_2-$, $SiCH_3PO_4-$, $C(O)-$ and $S(O)_2-$;

X^3 is selected from the group consisting of $-C(O)H$, $-CO_2H$, $-CH_3$, $-C(CH_3)_3$, $-Si(CH_3)_3$, $-SiCH_3(C(CH_3)_3)_2$, $-Si(C(CH_3)_3)_3$, $-Si(PO_4)_2C(CH_3)_3$, a phenyl group, an alkyl-substituted phenyl group having from 1 to 6 carbons in the alkyl chain, an alkyl chain having from 1 to 6 carbons, an amino moiety, a chlorine, a fluorine, or a group having the formula $C(R^3R^4)OH$, wherein each of R^3 and R^4 is independently an alkyl chain having from 1 to 6 carbons, a phenyl group or an alkyl-substituted phenyl group having from 1 to 6 carbons in the alkyl chain;



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wherein when Z^2 is an amino group, R^2 is an aliphatic chain having from 1 to 9 or from 19 to 23 carbon atoms in the aliphatic chain.

17. The compound of claim 16, wherein R^2 is an alkyl chain.

18. The compound of claim 16, wherein R^1 is $\text{CH}_3(\text{CH}_2)_{12}-$.

19. The compound of claim 16, wherein Y^1 is $-\text{CH}=\text{CH}-$.

20. The compound of claim 16, wherein Y^2 is H.

21. The compound of claim 16, wherein Y^3 is $-\text{C}(\text{O})\text{R}^2$.

22. The compound of claim 16, wherein Z^1 is OH.

23. The compound of claim 22, wherein Z^2 is a group having the formula $-\text{X}^2\text{X}^3$ or $\text{O}-\text{X}^2\text{X}^3$.

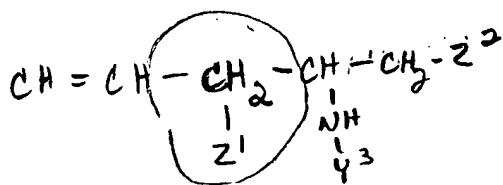
24. The compound of claim 23, wherein Z^2 is $-\text{OC}(\text{O})\text{CH}_3$, $-\text{OC}(\text{O})\text{CH}_2\text{CH}_2\text{CH}_3$, $-\text{OC}(\text{O})\text{CH}(\text{CH}_3)\text{CH}_3$, or $-\text{OSi}(\text{CH}_3)_2\text{C}(\text{CH}_3)_3$.

25. The compound of claim 24, wherein Z^2 is $-\text{OSi}(\text{CH}_3)_2\text{C}(\text{CH}_3)_3$.

26. The compound of claim 22, wherein Z^2 is a group having the formula $-\text{X}^1$ or OX^1 .

27. The compound of claim 16 having the formula $\text{CH}_3(\text{CH}_2)_{12}-\text{CH}=\text{CH}-\text{CH}_2\text{Z}^1-\text{CH}(\text{NH}Y^3)-\text{CH}_2-\text{Z}^2$.

this gives carbon a valence of 5



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28. The compound of claim 27, wherein Z^1 is OH and Y^3 is a group having the formula $-C(O)R^2$.
29. The compound of claim 28, wherein Y^3 is $-C(O)(CH_2)_4CH_3$.
30. The compound of claim 27, wherein Z^2 is $-OSi(CH_3)_2C(CH_3)_3$, $-OSi(PO_4)_2C(CH_3)_3$, $-C(O)CH_3$ or $-OC(O)CH_2CH_2CH_3$.
31. A pharmaceutical composition comprising the compound of claim 16.
32. A liposome having a bilayer comprising a lipid component, said lipid component comprising at least about 5 mole percent of the compound of claim 16.

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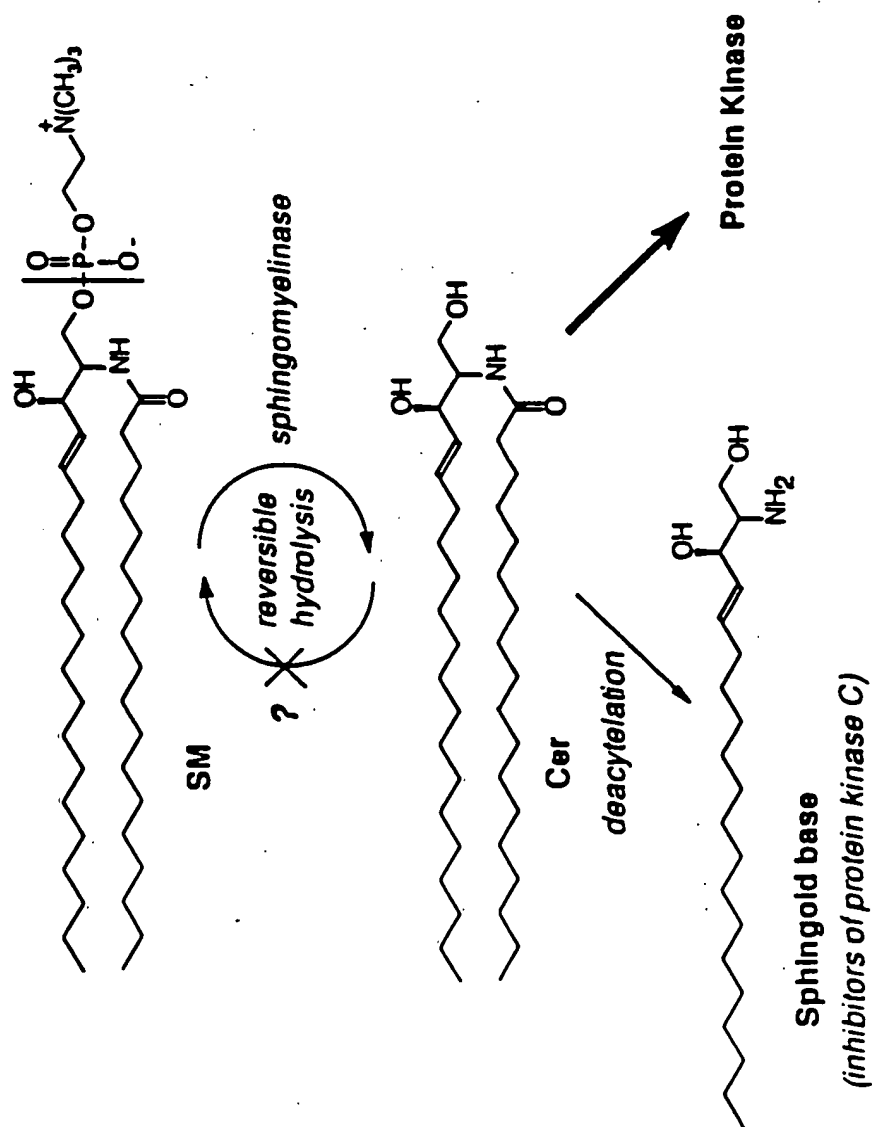
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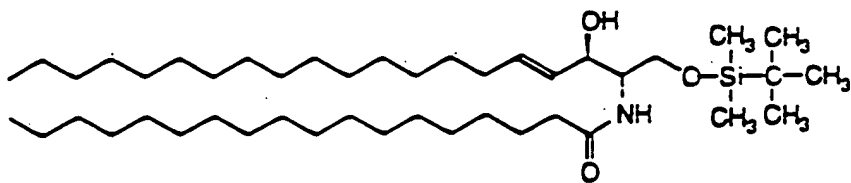
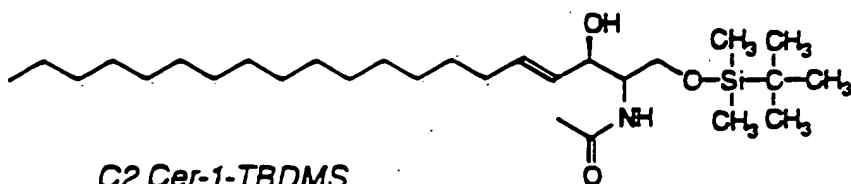
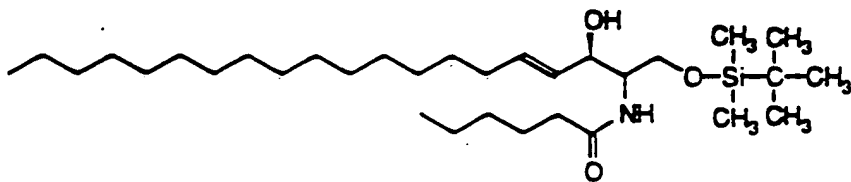
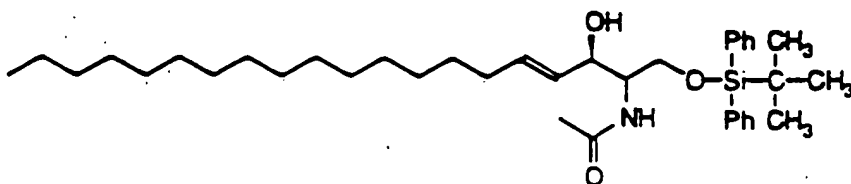
APPROVED	O.G. FIG. 3
BY	CLASS
DRAFTSMAN	424
	450

Fig. 1



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Fig. 2a

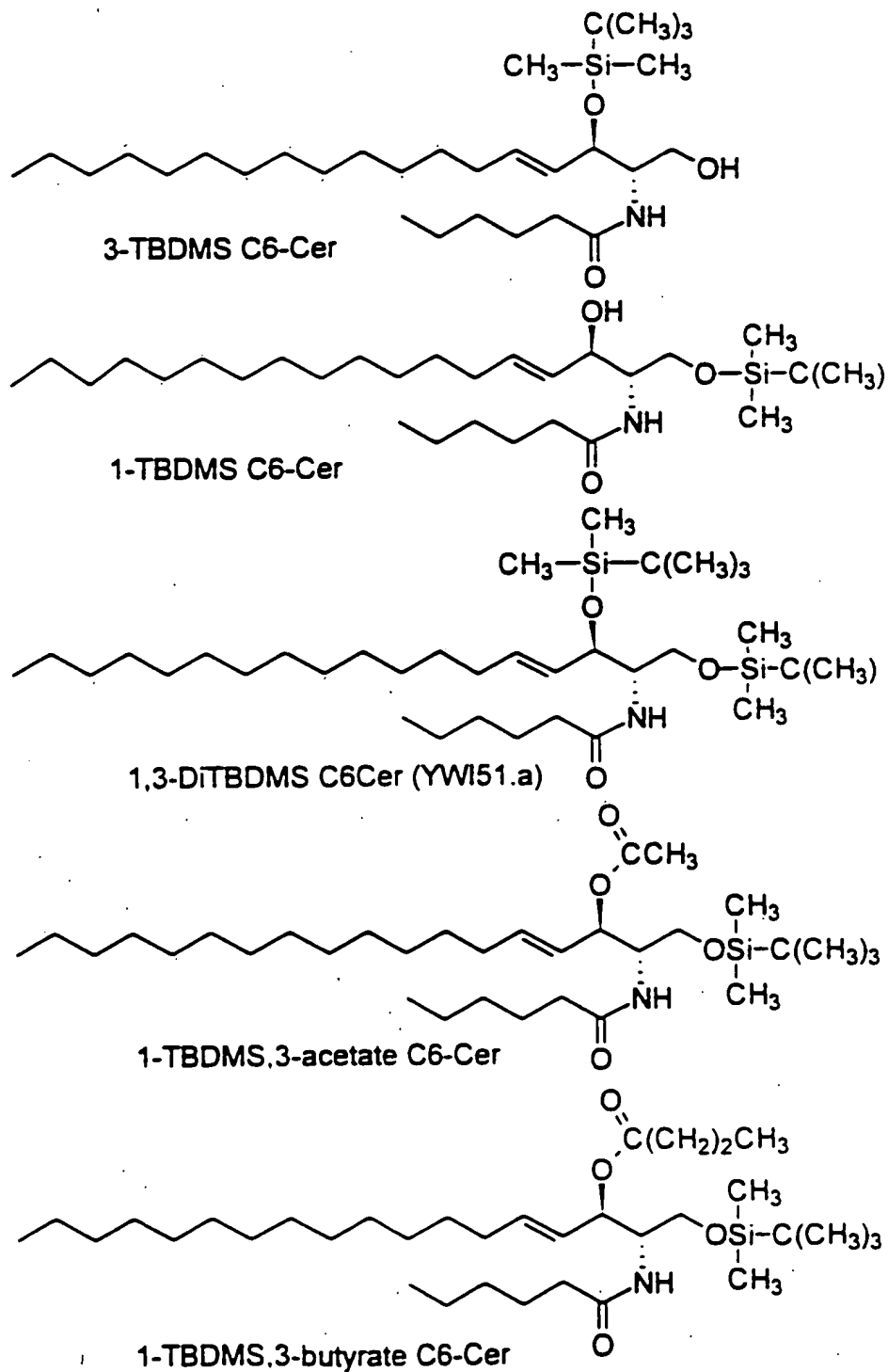
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APPROVED	O.G. FIG.	
	CLASS	SUBCLASS
BY		
DRAFTSMAN		

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Fig. 2b

APPROVED	O.G. FIG.
BY	CLASS SUBCLASS
DRAFTSMAN	

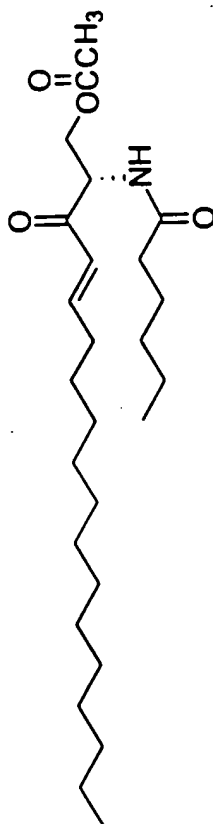


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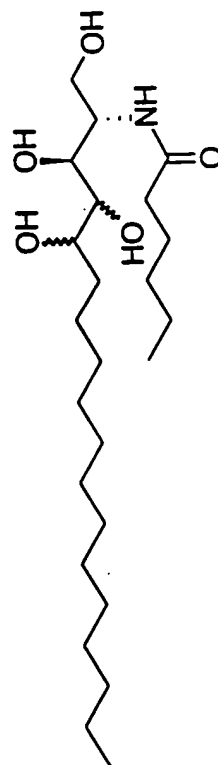
APPROVED	O.G. FIG.
BY	CLASS
DRAFTSMAN	SUBCLASS

4/21

Fig. 2c



1-Acetate-3-one C6-Ce.



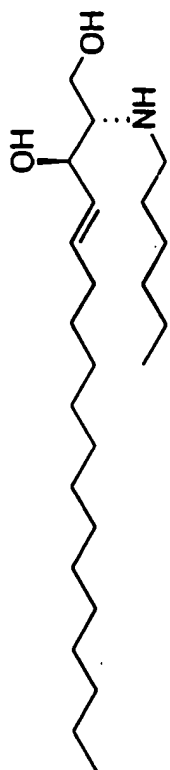
4,5-Diol C6-Cer

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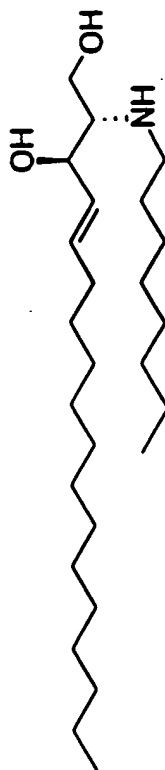
APPROVED	O.G. FIG.
BY	CLASS
DRAFTSMAN	SUBCLASS

5/21

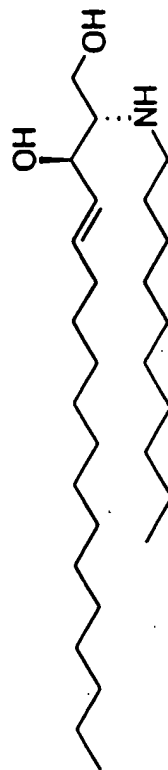
Fig. 2d



N-Hexyl Sphingosine (or N-C6 Sphingosine)



N-C8 Sphingosine



N-C10 Sphingosine

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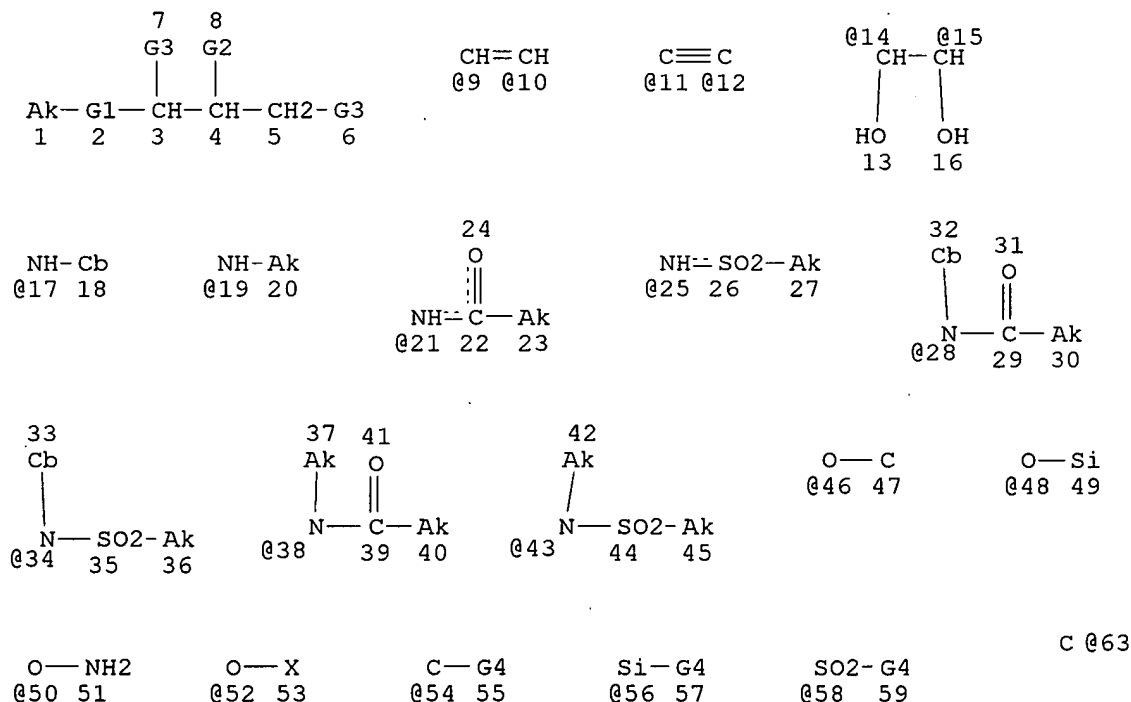
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Structure search limits have been increased. See HELP SLIMIT
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L2 STR

Full file search done on this structure.



Page 1-A

O-G5-G4
 @60 61 62

Page 2-A

VAR G1=9-1 10-3/11-1 12-3/14-1 15-3
 VAR G2=NH2/17/19/21/25/28/34/38/43
 VAR G3=OH/63/SI/NH2/X/46/48/50/52/54/56/58/60
 VAR G4=63/SI/NH2/X
 VAR G5=C/SI/SO2
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 CONNECT IS E1 RC AT 1

Searched by Barb O'Bryen & Toby Port

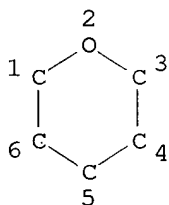
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CONNECT IS E1 RC AT 23
CONNECT IS E1 RC AT 27
CONNECT IS E1 RC AT 30
CONNECT IS E1 RC AT 36
CONNECT IS E1 RC AT 37
CONNECT IS E1 RC AT 40
CONNECT IS E1 RC AT 42
CONNECT IS E1 RC AT 45
DEFAULT MLEVEL IS ATOM
GGCAT IS MCY UNS AT 18
GGCAT IS MCY UNS AT 32
GGCAT IS MCY UNS AT 33
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS E6 C AT 18
ECOUNT IS E6 C AT 32
ECOUNT IS E6 C AT 33

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GRAPH ATTRIBUTES:
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 NUMBER OF NODES IS 63

STEREO ATTRIBUTES: NONE
 L3 STR



← this structure NOTED out of full file answer set.

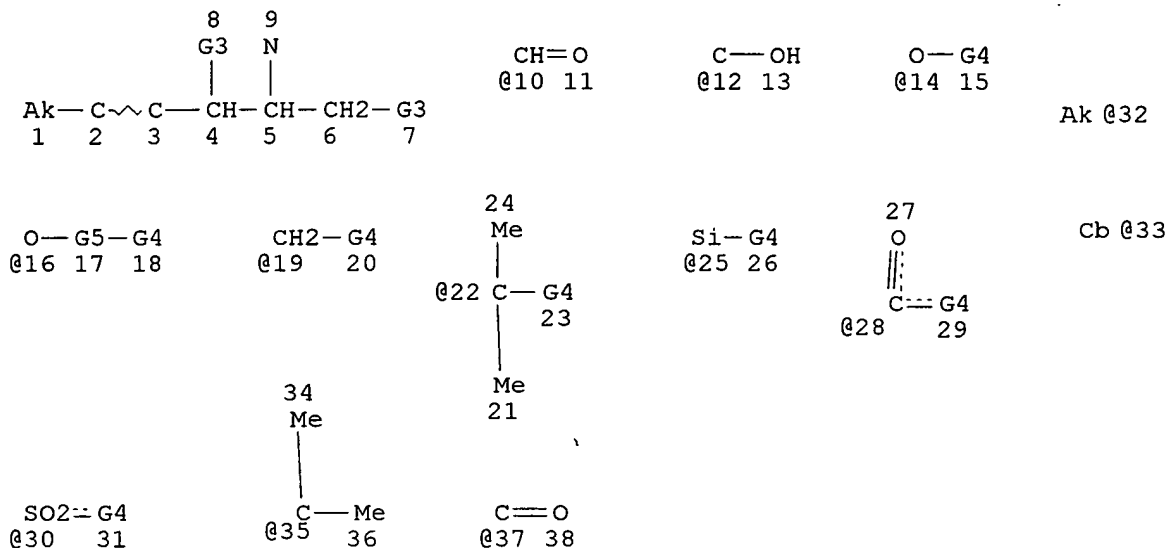
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STEREO ATTRIBUTES: NONE

L4 983 SEA FILE=REGISTRY SSS FUL L2 NOT L3
 L7 STR

sub file search done on this structure, shown on page 3
 Z1 + Z2 more specifically defined.



VAR G3=OH/10/COOH/32/SI/33/NH2/X/12/14/16/19/22/25/28/30

VAR G4=10/COOH/32/SI/33/NH2/X/12

VAR G5=CH2/35/SI/37/SO2

NODE ATTRIBUTES:

CONNECT IS E1 RC AT 32

DEFAULT MLEVEL IS ATOM

GGCAT IS LIN AT 1

GGCAT IS MCY UNS AT 33

DEFAULT ECLEVEL IS LIMITED

ECOUNT IS M5-X19 C AT 1

ECOUNT IS E6 C AT 33

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

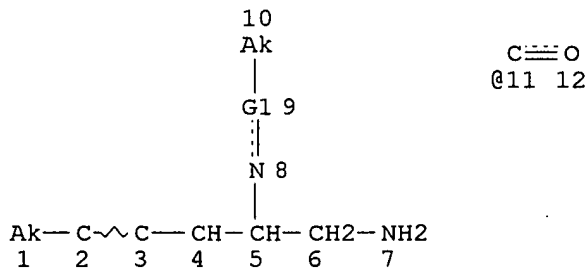
NUMBER OF NODES IS 38

STEREO ATTRIBUTES: NONE

L10 650 SEA FILE=REGISTRY SUB=L4 SSS FUL L7

L15 STR

*This structure addresses the proviso at the end of claim 16.
Z2 = NH2. and R2 = AK.*



VAR G1=11/SO2

NODE ATTRIBUTES:

CONNECT IS E1 RC AT 10

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 12

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STEREO ATTRIBUTES: NONE

L17 3 SEA FILE=REGISTRY SUB=L10 SSS FUL L15

100.0% PROCESSED 3 ITERATIONS

3 ANSWERS

SEARCH TIME: 00.00.01

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L3 STR
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L7 STR
L10 650 SEA FILE=REGISTRY SUB=L4 SSS FUL L7
L15 STR
L17 3 SEA FILE=REGISTRY SUB=L10 SSS FUL L15
L18 1 SEA FILE=CAPLUS ABB=ON PLU=ON L17

=> d ibib abs hitstr l18 1; file caold; d que nos l19

L18 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 2000:199315 CAPLUS

DOCUMENT NUMBER: 132:236933

TITLE: Preparation of sphingomyelinase-inhibiting ceramide analogs

INVENTOR(S): Kiso, Makoto; Ishida, Shuji

PATENT ASSIGNEE(S): Ohtsuka Pharmaceutical Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 13 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

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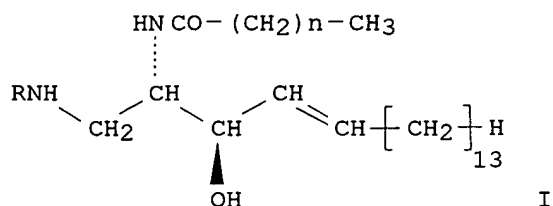
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2000086601	A2	20000328	JP 1998-251197	19980904

OTHER SOURCE(S): MARPAT 132:236933

GI



AB Ceramide analogs I [R = H, (halo)alkoxycarbonyl; n = 0-22] or their salts are prepd. I show sphingomyelinase inhibition, ceramide glucosylation promotion, sphingosine acyltransferase inhibition, ceramide antagonism, etc., and are useful for treatment of dementia, memory disturbance, inflammation, etc. (no data). (2S,3R,4E)-2-acetylamino-1-azido-4-octadecen-3-ol (prepn. given) was treated with PPh₃ in C₆H₆/H₂O at 55.degree. for 3 h to give 75% I (R = H, n = 0).

IT 262288-84-6P 262288-85-7P 262288-86-8P

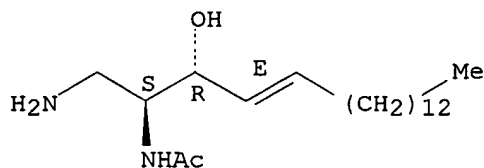
RL: RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of sphingomyelinase-inhibiting ceramides)

RN 262288-84-6 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-1-(aminomethyl)-2-hydroxy-3-heptadecenyl]- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

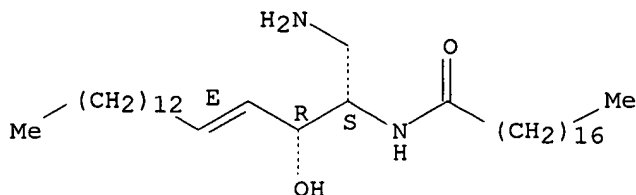


RN 262288-85-7 CAPLUS

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Absolute stereochemistry.

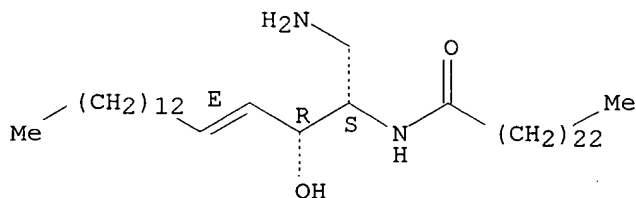
Double bond geometry as shown.



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RN 262288-86-8 CAPLUS
 CN Tetracosanamide, N-[(1S,2R,3E)-1-(aminomethyl)-2-hydroxy-3-heptadecenyl]-
 (9CI) (CA INDEX NAME)

Absolute stereochemistry.
 Double bond geometry as shown.



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L7          STR
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L15         STR
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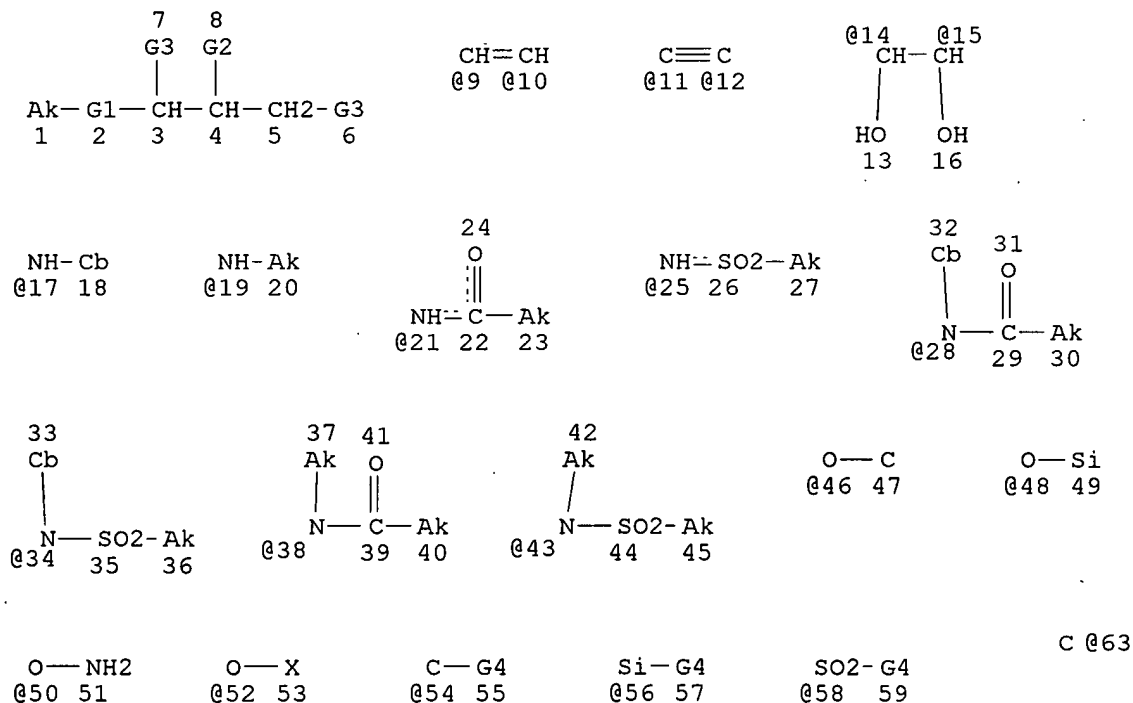
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 for details.

L2

STR

This structure is the full file search.



Page 1-A

$$\begin{array}{c} \text{O}-\text{G5}-\text{G4} \\ @60 \quad 61 \quad 62 \end{array}$$

Page 2-A

VAR G1=9-1 10-3/11-1 12-3/14-1 15-3
 VAR G2=NH2/17/19/21/25/28/34/38/43
 VAR G3=OH/63/SI/NH2/X/46/48/50/52/54/56/58/60
 VAR G4=63/SI/NH2/X
 VAR G5=C/SI/SO2

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NSPEC IS RC AT 47
 NSPEC IS RC AT 63

Searched by Barb O'Bryen & Toby Port

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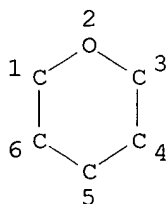
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CONNECT IS E1 RC AT 42
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DEFAULT MLEVEL IS ATOM
GGCAT IS MCY UNS AT 18
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DEFAULT ECLEVEL IS LIMITED
ECOUNT IS E6 C AT 18
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STEREO ATTRIBUTES: NONE
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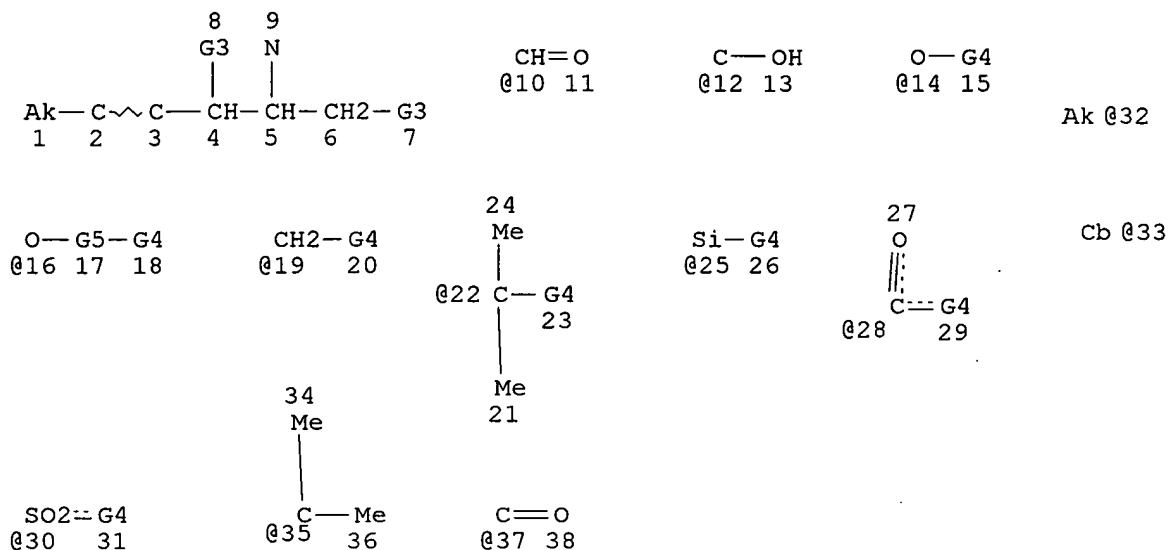


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L7 STR *Subfile search done on this structure, shown on page 9.*
Z1 + Z2 more specifically defined



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VAR G4=10/COOH/32/SI/33/NH2/X/12

VAR G5=CH2/35/SI/37/SO2

NODE ATTRIBUTES:

CONNECT IS E1 RC AT 32

DEFAULT MLEVEL IS ATOM

GGCAT IS LIN AT 1

GGCAT IS MCY UNS AT 33

DEFAULT ECLEVEL IS LIMITED

ECOUNT IS M5-X19 C AT 1

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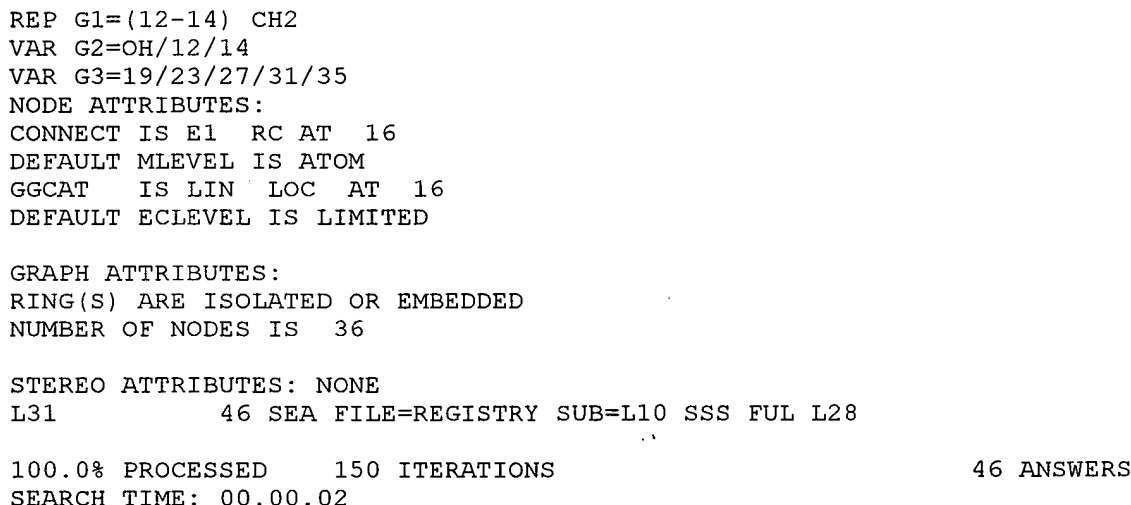
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STEREO ATTRIBUTES: NONE

L10 650 SEA FILE=REGISTRY SUB=L4 SSS FUL L7

L28 STR

L10 has too many answers, so structure L28 further narrows the answer set. Definitions from claims 18, 19, 20, 21, 22, 24, 25+30 are used to further define the structure of L28.



FILE 'CAPLUS' ENTERED AT 16:04:35 ON 07 JUL 2000
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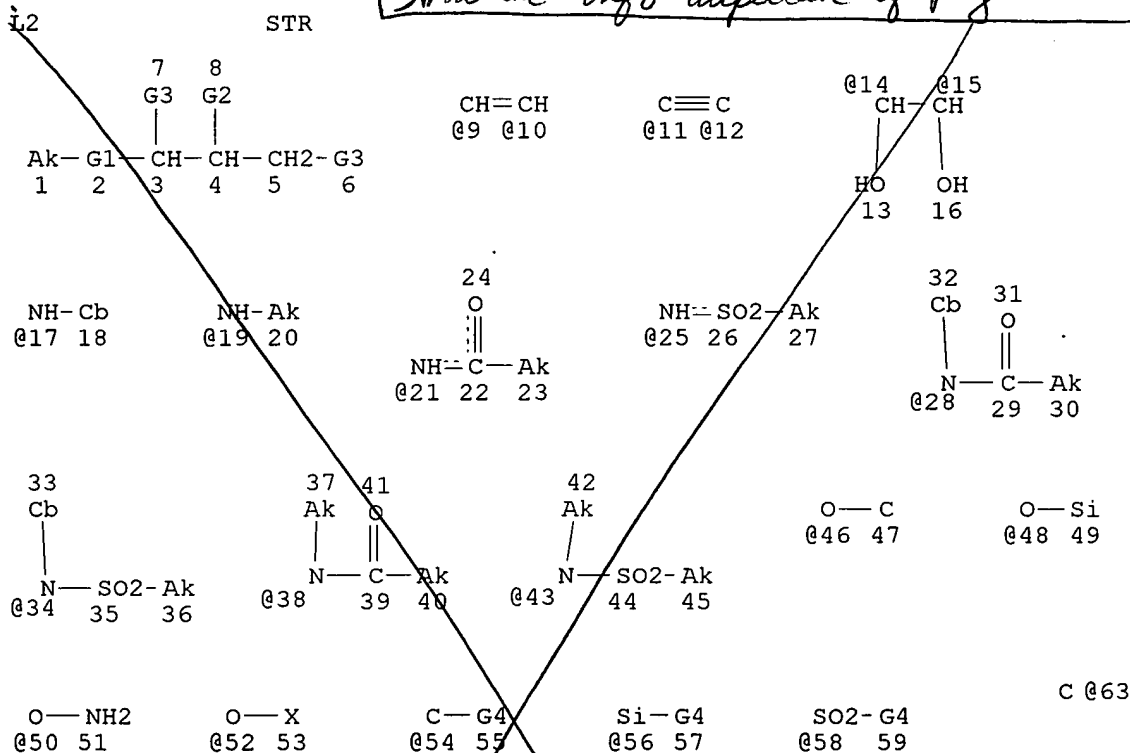
FILE COVERS 1967 - 7 Jul 2000 VOL 133 ISS 2
FILE LAST UPDATED: 6 Jul 2000 (20000706/ED)
Searched by Barb O'Bryen & Toby Port

This file contains CAS Registry Numbers for easy and accurate substance identification.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

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Structure info duplicate of pages 7-10



Page 1-A

O-G5-G4
@60 61 62

Page 2-A

VAR G1=9-1 10-3/11-1 12-3/14-1 15-3
VAR G2=NH2/17/19/21/25/28/34/38/43
VAR G3=OH/63/SI/NH2/X/46/48/50/52/54/56/58/60
VAR G4=63/SI/NH2/X
VAR G5=C/SI/SO2

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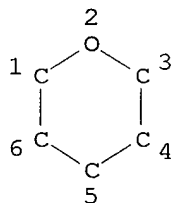
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CONNECT	IS	E1	RC	AT 1
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CONNECT	IS	E1	RC	AT 23
CONNECT	IS	E1	RC	AT 27
CONNECT	IS	E1	RC	AT 30
CONNECT	IS	E1	RC	AT 36

Searched by Barb O'Bryen & Toby Port

CONNECT IS E1 RC AT 37
 CONNECT IS E1 RC AT 40
 CONNECT IS E1 RC AT 42
 CONNECT IS E1 RC AT 45
 DEFAULT MLEVEL IS ATOM
 GGCAT IS MCY UNS AT 18
 GGCAT IS MCY UNS AT 32
 GGCAT IS MCY UNS AT 33
 DEFAULT ECLEVEL IS LIMITED
 ECOUNT IS E6 C AT 18
 ECOUNT IS E6 C AT 32
 ECOUNT IS E6 C AT 33

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 63

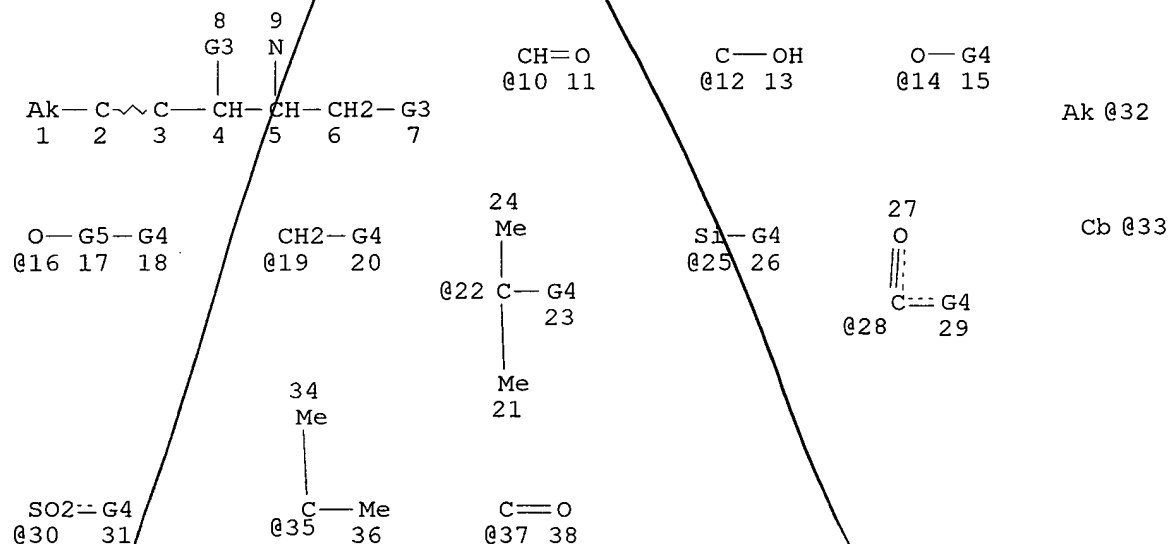
STEREO ATTRIBUTES: NONE
 L3 STR



NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RSPEC I
 NUMBER OF NODES IS 6

STEREO ATTRIBUTES: NONE
 L4 983 SEA FILE=REGISTRY SSS FUL L2 NOT L3
 L7 STR



VAR G3=OH/10/COOH/32/SI/33/NH2/X/12/14/16/19/22/25/28/30
 VAR G4=10/COOH/32/SI/33/NH2/X/12

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VAR G5=CH2/35/SI/37/SO2

NODE ATTRIBUTES:

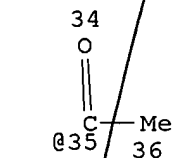
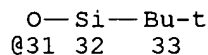
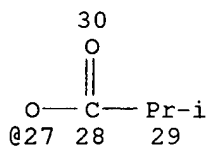
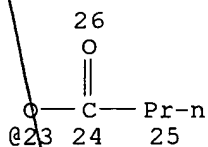
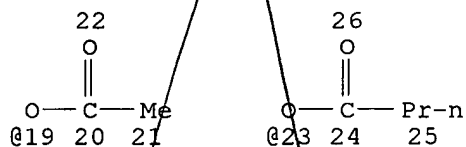
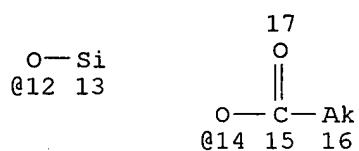
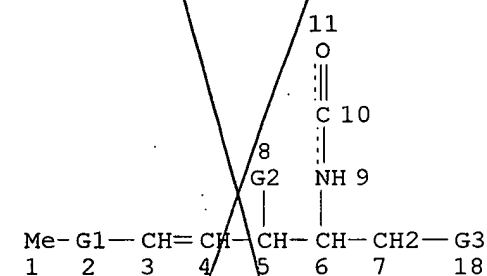
CONNECT IS E1 RC AT 32
 DEFAULT MLEVEL IS ATOM
 GGCAT IS LIN AT 1
 GGCAT IS MCY UNS AT 33
 DEFAULT ECLEVEL IS LIMITED
 ECOUNT IS M5-X19 C AT 1
 ECOUNT IS E6 C AT 33

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 38

STEREO ATTRIBUTES: NONE

L10 650 SEA FILE=REGISTRY SUB=L4 SSS FUL L7
 L28 STR



REP G1=(12-14) CH2

VAR G2=OH/12/14

VAR G3=19/23/27/31/35

NODE ATTRIBUTES:

CONNECT IS E1 RC AT 16
 DEFAULT MLEVEL IS ATOM
 GGCAT IS LIN LOC AT 16
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 36

STEREO ATTRIBUTES: NONE

L31 46 SEA FILE=REGISTRY SUB=L10 SSS FUL L28
 L32 72 SEA FILE=CAPLUS ABB=ON PLU=ON L31

=> d ibib abs hitstr l32 1-72; file caold; dque nos l33

Searched by Barb O'Bryen & Toby Port

L32 ANSWER 1 OF 72 CAPLUS COPYRIGHT 2000 ACS

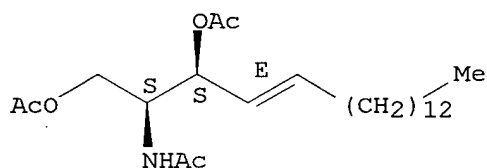
ACCESSION NUMBER: 2000:128525 CAPLUS
 DOCUMENT NUMBER: 132:293951
 TITLE: A chemoenzymatic access to D- and L-sphingosines employing hydroxynitrile lyases
 AUTHOR(S): Johnson, Dean V.; Felfer, Ulfried; Griengl, Herfried
 CORPORATE SOURCE: Spezialforschungsbereich Biokatalyse, Institut für Organische Chemie der Technischen Universität Graz, Graz, A-8010, Austria
 SOURCE: Tetrahedron (2000), 56(5), 781-790
 CODEN: TETRAB; ISSN: 0040-4020
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB A chemoenzymic access to D- or L-sphingosines is presented comprising of a total synthesis of the L-threo-isomer and formal syntheses of the other three isomers. Key to the development of a general synthetic strategy has been the use of enantio-complementary hydroxynitrile lyases (Hnls) to yield an enantiomeric pair of starting materials. The (S)-Hnl from *Hevea brasiliensis* has been used to prep. L-threo-sphingosine in 14 steps and an overall 12% yield. Application of the (R)-Hnl from *Prunus amygdalus* formally allows synthesis of D-threo- and D-erythro-sphingosines.

IT **78779-96-1P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (chemoenzymic access to D- and L-sphingosines employing hydroxynitrile lyases)

RN 78779-96-1 CAPLUS
 CN Acetamide, N-[(1S,2S,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
 Double bond geometry as shown.



REFERENCE COUNT: 53
 REFERENCE(S):
 (1) Albrecht, J; Biotechnol Appl Biochem 1993, V17, P191 CAPLUS
 (2) Baker, R; J Chem Soc, Perkin Trans 1 1989, P190 CAPLUS
 (3) Borek, C; Proc Natl Acad Sci USA 1991, V88, P1953 CAPLUS
 (4) Brussee, J; Tetrahedron 1990, V46, P979 CAPLUS
 (5) Brussee, J; Tetrahedron 1990, V46, P979 CAPLUS
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 2 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1999:787651 CAPLUS
 DOCUMENT NUMBER: 132:18776
 TITLE: Preparation of fat emulsions which contains the ceramide derivatives as cancer metastasis inhibitors
 INVENTOR(S): Mizushima, Hiroshi; Igarashi, Toshisato; Mizushima, Noboru; Takenaga, Mitsuko; Morisawa, Yoshitomi; Nakayama, Toshiaki
 PATENT ASSIGNEE(S): LTT Inst. Co., Ltd., Japan; Asahi Glass Co., Ltd.
 Searched by Barb O'Bryen & Toby Port

SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11343249	A2	19991214	JP 1998-150128	19980529

OTHER SOURCE(S): MARPAT 132:18776

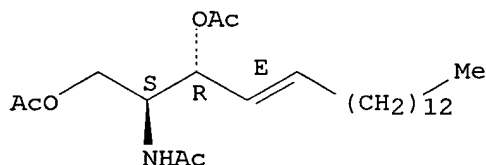
AB Fat emulsions which contains the ceramide derivs. (Markush's structure given) are claimed as cancer metastasis inhibitors. The antimetastatic effect of the ceramide derivs. was tested in mice.

IT **2482-37-3P**
 RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (CeRa-03; prepn. of fat emulsions which contains the ceramide derivs. as cancer metastasis inhibitors)

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).
 Double bond geometry as shown.



L32 ANSWER 3 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1999:712892 CAPLUS

DOCUMENT NUMBER: 132:212571

TITLE: Lipid microsphere preparation of a lipophilic ceramide derivative suppressed the colony formation of murine experimental metastasis

AUTHOR(S): Takenaga, Mitsuko; Igarashi, Rie; Matsumoto, Kayo; Mizushima, Noboru; Nakayama, Toshiaki; Mizushima, Yutaka

CORPORATE SOURCE: The Second Department of the Institute of Medical Science, St. Marianna University School of Medicine, Kanagawa, 216-8512, Japan

SOURCE: Drug Delivery Syst. (1999), 14(5), 373-379
 CODEN: DDSYEI; ISSN: 0913-5006

PUBLISHER: Nippon DDS Gakkai Jimukyoku

DOCUMENT TYPE: Journal

LANGUAGE: Japanese

AB Ceramide is well known as a regulator of cell apoptosis and cell growth suppression. In this study, we synthesized more lipophilic ceramide derivs. in order to incorporate into lipid microsphere (LM), and their activity was evaluated in vivo. Cera 03, a diacetylated form of C2-ceramide showed a potent cell growth inhibition and potently induced apoptosis in both U 937 cells and Meth A-T tumor cells in vitro, with a similar potency as cell membrane-permeable C2-ceramide. Diacetylated form of natural type ceramide (Cer), Cera 02, also suppressed the in vitro cell growth with a similar potency as that of Cer, which was much lower than

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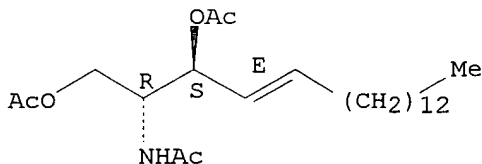
IT 67113-24-0P

(lipid microsphere prepn. of a lipophilic ceramide deriv. suppressed colony formation of murine exptl. metastasis)

RN 67113-24-0 CAPLUS

Relative stereochemistry.

Double bond geometry as shown.



L32 ANSWER 4 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1999:672566 CAPLUS

DOCUMENT NUMBER: 131:295576

TITLE: Spisulosine compounds having antitumor activity

INVENTOR(S): Rinehart, Kenneth Lloyd; Fregeau, Nancy Louise;
Warwick, Robert Arthur; Garcia Gravalos, Dolores;
Avila, Jesus; Faircloth, Glynn Thomas

PATENT ASSIGNEE(S): The Board of Trustees of the University of Illinois,
USA; Ruffles, Graham, Keith

SOURCE: PCT Int. Appl., 73 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9952521	A1	19991021	WO 1999-GB1091	19990409
W:	AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			

PRIORITY APPLN. INFO.: US 1998-58456 19980410

AB Investigation of the activity of exts. of the clam *Spisula polynyma* has led to antitumor long-chain, straight-chain alkane or alkene compds. which
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have a 2-amino group and a 3-hydroxy group.

IT 2482-37-3P

RL: BOC (Biological occurrence); PUR (Purification or recovery); SPN (Synthetic preparation); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)

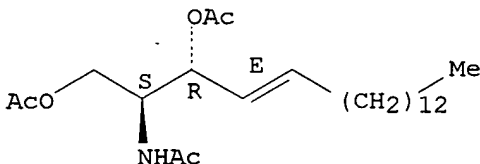
(spisulosine compds. having antitumor activity)

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

Double bond geometry as shown.



REFERENCE COUNT: 7

REFERENCE(S):

- (1) Bell, R; US 4816450 A 1989
- (2) Biomembrane Inst; EP 0381514 A 1990
- (3) Biomembrane Inst; WO 9618404 A 1996
- (4) Kinkade, J; US 5190876 A 1993
- (6) Shallenberger, R; EXPERIENTIA 1974, V30(6), P597

CAPLUS

ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 5 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1999:476763 CAPLUS

DOCUMENT NUMBER: 131:286282

TITLE: A short enantiodivergent synthesis of D-erythro and L-threo sphingosine

AUTHOR(S): Khlar, Nouredine; Singh, Kamaljit; Garcia, Mercedes; Martin-Lomas, Manuel

CORPORATE SOURCE: Grupo de Carbohidratos, Instituto de Investigaciones Quimicas, C.S.I.C., Seville, 41092, Spain

SOURCE: Tetrahedron Lett. (1999), 40(31), 5779-5782

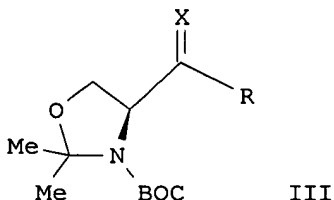
CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



III

AB A new, short (6 steps) and efficient enantiodivergent route to both D-erythro and L threo-sphingosine I and II [HOCH₂CH(NH₂)CH(OH)CH=CH(CH₂)₁₂Me] is disclosed. The high diastereoselection (100% de) reached in the creation of the C-3 stereocenter relies on the use of a sulfoxide as chiral controlling agent in the redn. of the common precursor

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(R)-.beta.-keto sulfoxide (III) (R = S(=O)-4-Me-C₆H₄, X = =O). The desired E-alkene of sphingosines has been constructed by the Schlosser modification of the Wittig reaction between the aldehyde III (R = CHO, X = .alpha.OCH₂OMe) (IV) and the phosphonium salt Me(CH₂)₁₂PPH₃Br. The reported methodol. can easily be extended to the synthesis of a large no. of optically pure syn and anti amino alcs. starting from com. available amino acids.

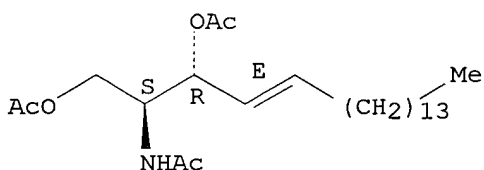
IT 246245-48-7P 246245-49-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(enantiodivergent synthesis of D-erythro and L-threo sphingosine)

RN 246245-48-7 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-octadecenyl]- (9CI) (CA INDEX NAME)

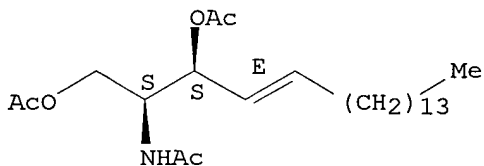
Absolute stereochemistry.
Double bond geometry as shown.



RN 246245-49-8 CAPLUS

CN Acetamide, N-[(1S,2S,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-octadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



REFERENCE COUNT:

28

REFERENCE(S):

- (1) Arnone, A; J Org Chem 1996, V61, P3375 CAPLUS
- (3) Carreno, M; Chem Rev 1995, V95, P1717 CAPLUS
- (4) Carreno, M; J Org Chem 1990, V55, P2120 CAPLUS
- (5) Dietrich, H; Chemistry Eur J 1999, V5, P320 CAPLUS
- (7) Enders, D; Chem Eur J 1995, V1, P382 CAPLUS

ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 6 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1998:758649 CAPLUS

DOCUMENT NUMBER: 130:66723

TITLE: Preparation of digalactosyl ceramides and their intermediates

INVENTOR(S): Nakahon, Kazutaka

PATENT ASSIGNEE(S): Eisai Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 11 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

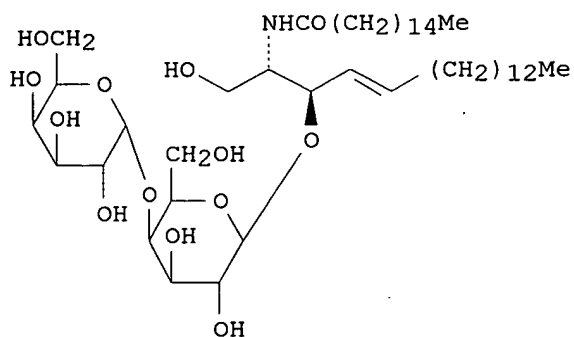
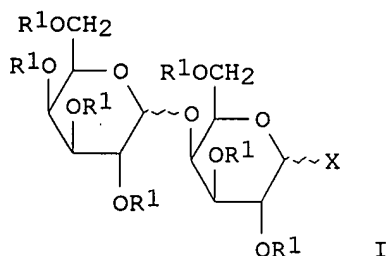
PATENT INFORMATION:

Searched by Barb O'Bryen & Toby Port

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 10310596	A2	19981124	JP 1997-119195	19970509

OTHER SOURCE(S): CASREACT 130:66723; MARPAT 130:66723

GI



AB Title compds. I [R1 = H; X = OR; wherein R = CH₂CH(NHCOR₂)CH(OR₃)CH:CH(CH₂)₁₂Me, CH[CH(CH₂OR₃)NHCOR₂]CH:CH(CH₂)₁₂Me; R₂ = pentadecanyl, heptadecanyl, 8-heptadecenyl; R₃ = H] are prepd. by reaction of halides I (X = halo; R1 = protective group) with ROH (R = same as I; R₃ = protective group) and deprotection of I (R1 = protective group; X = OR; wherein CH₂CH(NHCOR₂)CH(OR₃)CH:CH(CH₂)₁₂Me, CH[CH(CH₂OR₃)NHCOR₂]CH:CH(CH₂)₁₂Me; R₃ = protective group). The deprotected I are useful as anticancer agents, immunosuppressants, anti-HIV agents, detoxicants, Gaucher disease inhibitors (no data). .beta.(1.fwdarw.4)-I (R1 = Ac, X = F) (prepn. given) was treated with (2S,3R,4E)-1-O-benzoyl-2-N-palmitoylsphingosine (prepn. given) in CH₂Cl₂ in the presence of AgClO₄, TiCl₄, and mol. sieve 4A at 0.degree. for 17 h to give 12% protected digalactosyl ceramide, which was deprotected by MeONa in MeOH-THF at room temp. for 90 min to give 72% the title compd. (II).

IT 143517-08-2P

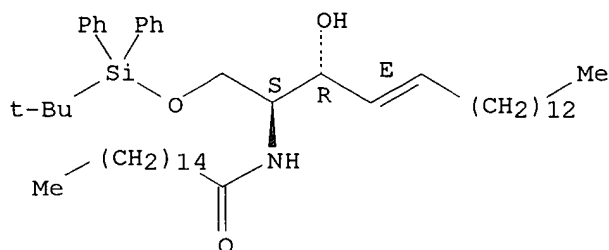
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of digalactosyl ceramides as pharmaceuticals)

RN 143517-08-2 CAPLUS

CN Hexadecanamide, N-[(1S,2R,3E)-1-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]methyl]-2-hydroxy-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

Double bond geometry as shown.



L32 ANSWER 7 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1998:85260 CAPLUS

DOCUMENT NUMBER: 128:101927

TITLE: Chemoenzymic synthesis of all four stereoisomers of sphingosine from chlorobenzene: glycosphingolipid precursors

AUTHOR(S): Nugent, Thomas C.; Hudlicky, Tomas

CORPORATE SOURCE: Dep. Chem., Univ. Florida, Gainesville, FL, 32611-7200, USA

SOURCE: J. Org. Chem. (1998), 63(3), 510-520

CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 128:101927

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Advantageous use of homochiral cyclohexadiene-cis-1,2-diol I,, available by means of biocatalytic oxidn. of chlorobenzene with toluene dioxygenase, has enabled the synthesis of all four enantiomerically pure C18-sphingosines II. The four requisite azido alc. diastereomers III were accessed by regioselective opening of stereoisomeric epoxides with either azide or halide ions. The configuration of C4 and C5 in azides III defines the stereochem. of the incipient sphingosine chain, liberated from by the oxidative cleavage of the C1-C6 olefin. For L-threo-sphingosine [(2S,3S)-II], lactol IV generated by this cleavage was converted by periodate oxidn. to azido deoxy L-threose V,, which gave (2S,3S)-II upon Wittig olefination and redn. Similarly, D-erythro-sphingosine [(2S,3R)-II] and L-erythro-sphingosine [(2R,3S)-II] were generated from (4S,5S)- and (4R,5R)-III, resp. The last sphingosine [(2R,3R)-II] was synthesized from the silyl-protected azido alc. VI. Subsequent transformations provided silyl-protected azido deoxy D-threose VII, which upon Wittig olefination and redn. gave D-threo-sphingosine [(2R,3R)-II]. Exptl. and spectral data are provided for all new compds.

IT 201340-32-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(chemoenzymic synthesis of all four sphingosine stereoisomers from chlorobenzene)

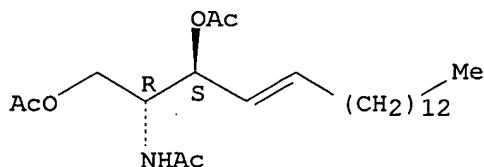
RN 201340-32-1 CAPLUS

CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

Searched by Barb O'Bryen & Toby Port



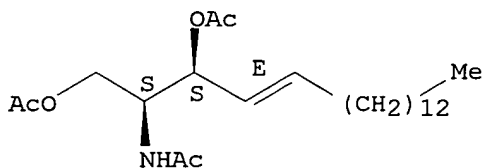
IT 78779-96-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
(chemoenzymic synthesis of all four sphingosine stereoisomers from chlorobenzene)

RN 78779-96-1 CAPLUS

CN Acetamide, N-[(1S,2S,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



L32 ANSWER 8 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1997:589524 CAPLUS

DOCUMENT NUMBER: 127:234526

TITLE: Improved, gram scale synthesis of N,O,O-triacetyl-erythro- and threo-C18-sphingosines from serine
AUTHOR(S): Dondoni, Alessandro; Perrone, Daniela; Turturici, Elisa

CORPORATE SOURCE: Laboratorio di Chimica Organica, Dipartimento di Chimica, Universita, Ferrara, 44100, Italy

SOURCE: J. Chem. Soc., Perkin Trans. 1 (1997), (16), 2389-2393
CODEN: JCPRB4; ISSN: 0300-922X

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 127:234526

AB A formal total synthesis of all four (E)-C18-sphingosine from serine has been carried out. This involves the thiazole-based homologation of the amino acid into a chiral 3-amino-2,4-dihydroxybutanal and the Wittig olefination with the ylide from the C14 alkyl phosphonium salt. The photoisomerization of the resulting mixt. of Z- and E-alkenes affords the target sphingosine. Thus, N,O,O-triacetyl-D-erythro C18-sphingosine and the L-threo isomer were prepd. in 43-44% overall yield from the N- and O-protected 3-amino-2,4-dihydroxybutanals. The corresponding antipodal L-erythro and D-threo isomers can be prepd. in the same way. Conversion of the above acetyl sphingosines into the free sphingoid bases has been reported in the literature.

IT 2482-37-3P 128387-01-9P 195194-55-9P

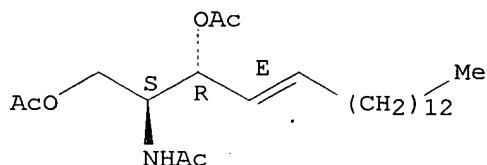
RL: SPN (Synthetic preparation); PREP (Preparation)
(improved gram scale prepn. of N,O,O-triacetyl-erythro- and threo-C18-sphingosines from serine)

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

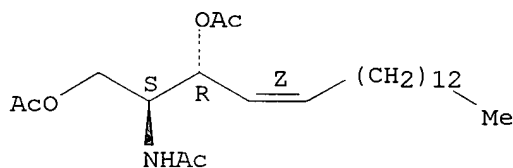
Searched by Barb O'Bryen & Toby Port

Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.



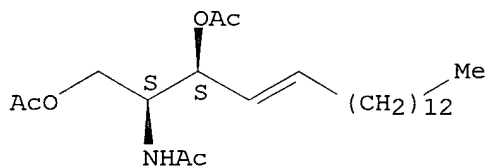
RN 128387-01-9 CAPLUS
CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-,
[R-[R*,S*-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.

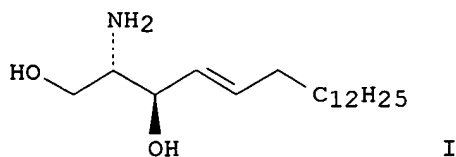


RN 195194-55-9 CAPLUS
CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-,
[S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



L32 ANSWER 9 OF 72 CAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1996:325160 CAPLUS
DOCUMENT NUMBER: 125:87046
TITLE: Synthesis of D-erythro-sphingosine from D-glucosamine
AUTHOR(S): Shinozaki, Katsuo; Mizuno, Kazuhiro; Masaki, Yukio
CORPORATE SOURCE: Gifu Pharmaceutical University, Gifu, 502, Japan
SOURCE: Chem. Pharm. Bull. (1996), 44(5), 927-932
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB D-Erythro-Sphingosine I was synthesized from D-glucosamine as a chiral pool through stereo-inversion of the C(3)-hydroxyl group via an oxidn.-redn. sequence, transformation to the erythro-amino-alc. chiron protected as the oxazolidinone, and elongation of the side chain at the C(6)-position.

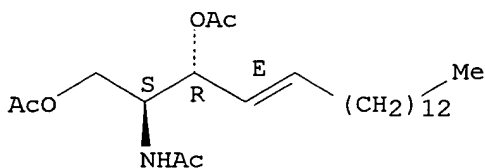
IT 2482-37-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of erythrosphingosine from glucosamine)

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.



L32 ANSWER 10 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1996:257368 CAPLUS

DOCUMENT NUMBER: 125:33996

TITLE: Synthetic studies on sphingolipids. 3. Efficient stereo controlled synthesis of D-erythro-sphingosine from N-benzoyl-D-glucosamine

AUTHOR(S): Murakami, Teiichi; Hato, Masakatsu

CORPORATE SOURCE: National Institute Materials Chemical Research, Tsukuba, 305, Japan

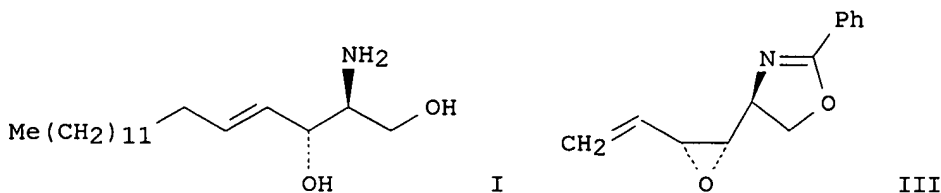
SOURCE: J. Chem. Soc., Perkin Trans. 1 (1996), (8), 823-7
CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 125:33996

GI



AB D-Erythro-sphingosine I is synthesized from 2-benzamido-2-deoxy-D-
Searched by Barb O'Bryen & Toby Port

glucopyranose (II) in a highly regio- and stereo-controlled manner. The key features in the synthesis involve the efficient conversion of II into the vinyl epoxide III and the subsequent SN2'-type reaction with a Grignard reagent in the presence of CuCN to afford the 1-O,2-N-protected sphingosine 11.

IT 2482-37-3P

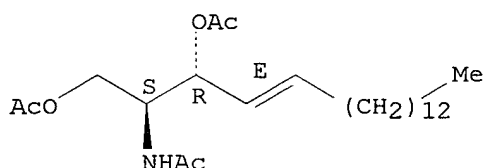
RL: SPN (Synthetic preparation); PREP (Preparation)
(asym. synthesis of erythrosphingosine from glucosamine)

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

Double bond geometry as shown.



L32 ANSWER 11 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1996:215544 CAPLUS

DOCUMENT NUMBER: 125:11289

TITLE: Enantiopure aminotriol from D-isoascorbic acid:
Synthesis of D-threo-C-18-sphingosine

AUTHOR(S): Tuch, Arounarith; Saniere, Michele; Le Merrer, Yves;
Depezay, Jean-Claude

CORPORATE SOURCE: Lab. Chim. Biochim., Pharmacologiques Toxicologiques,
Univ. Rene Descartes, Paris, 75270, Fr.

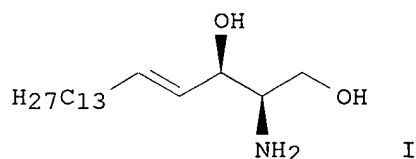
SOURCE: Tetrahedron: Asymmetry (1996), 7(3), 897-906

CODEN: TASYE3; ISSN: 0957-4166

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB Enantiopure suitably N,O-protected aminotriol has been prepd. from D-isoascorbic acid. The utility of this homochiral building block in the synthesis of D-threosphingosine I is described via a Wittig reaction on a N,O-protected .beta.-amino-.alpha.-hydroxyaldehyde.

IT 128387-05-3P

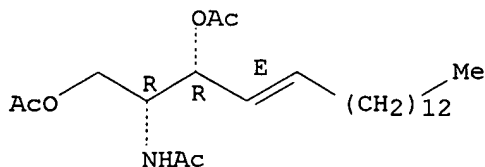
RL: SPN (Synthetic preparation); PREP (Preparation)
(enantiopure aminotriol from isoascorbic acid synthesis of
threosphingosine)

RN 128387-05-3 CAPLUS

CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-,
[R-[R*,R*-(E)]]- (9CI) (CA INDEX NAME)

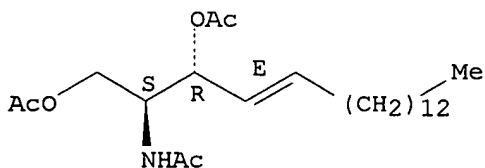
Searched by Barb O'Bryen & Toby Port

Absolute stereochemistry.
Double bond geometry as shown.



L32 ANSWER 12 OF 72 CAPLUS COPYRIGHT 2000 ACS
 ACCESSION NUMBER: 1996:190105 CAPLUS
 DOCUMENT NUMBER: 124:342900
 TITLE: Diastereoselective synthesis of triacetyl-L-erythro-C18-sphingosine
 AUTHOR(S): Miyata, Okiko; Yamaguchi, Sayaka; Ninomiya, Ichiya; Naito, Takeaki; Okamura, Kimio
 CORPORATE SOURCE: Kobe Pharmaceutical Univ., Higashinada, 658, Japan
 SOURCE: Chem. Pharm. Bull. (1996), 44(3), 636-8
 CODEN: CPBTAL; ISSN: 0009-2363
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 124:342900
 AB A new stereoselective synthetic route to triacetyl-L-erythro-C18-sphingosine has been developed by the combination of diastereoselective addn. of thiophenol to chiral olefins and subsequent intramol. substitution of the corresponding sulfonium group.
 IT **2482-37-3P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (stereoselective prepn. of triacetyl-L-erythro-C18-sphingosine)
 RN 2482-37-3 CAPLUS
 CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.

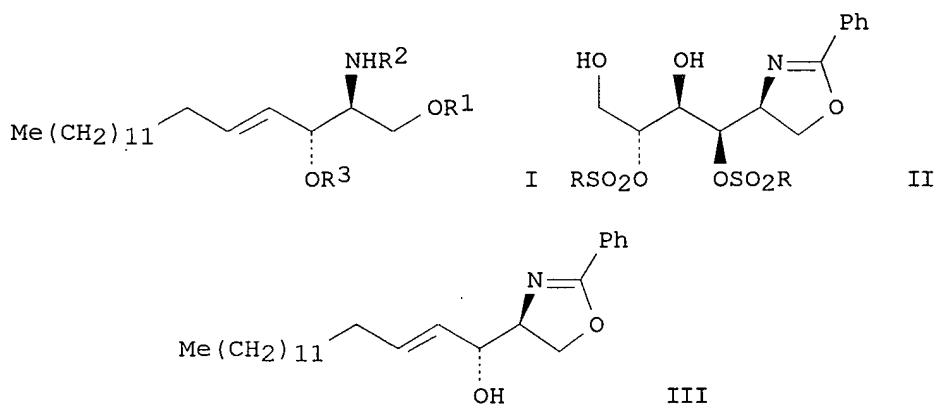


L32 ANSWER 13 OF 72 CAPLUS COPYRIGHT 2000 ACS
 ACCESSION NUMBER: 1996:113258 CAPLUS
 DOCUMENT NUMBER: 124:176808
 TITLE: Preparation of sphingosine derivatives
 INVENTOR(S): Murakami, Teiichi; Namikawa, Hiroyuki; Hado, Masakatsu
 PATENT ASSIGNEE(S): Kogyo Gijutsuin, Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

Searched by Barb O'Bryen & Toby Port

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 07258178	A2	19951009	JP 1994-74085	19940318
JP 2560250	B2	19961204		

OTHER SOURCE(S): CASREACT 124:176808; MARPAT 124:176808
GI



AB The title compds. I [R₁ - R₃ = H] are prep'd. in a multistep process. Thus, acetalization of N-benzoyl-D-glucosamine, followed by redn., sulfonylation, formation of oxazoline moiety, deacetalization, gave oxazoline derivs. II [R = alkyl]. II was converted in several steps to oxazoline deriv. III. III was treated with HCl in THF at room temp. for 20 h. NaOH, EtOH, and water were added to the reaction mixt. which was then stirred at 95.degree. for 16 h to give, after workup, I [R₁ = R₂ = R₃ = H].

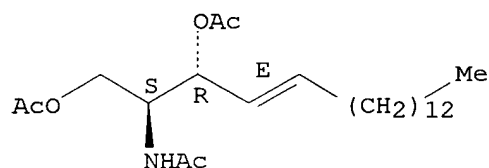
IT 2482-37-3P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of sphingosine derivs.)

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.



L32 ANSWER 14 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1995:958040 CAPLUS

DOCUMENT NUMBER: 124:768

TITLE: Pharmaceutically active sphingolipid compounds, liposomes containing them, and methods of use, especially for treatment of cancer

INVENTOR(S): Pei, Yong-Wei; Mayhew, Eric; Ahmad, Imran; Janoff, Andrew S.

PATENT ASSIGNEE(S): Liposome Co., Inc., USA
Searched by Barb O'Bryen & Toby Port

SOURCE: PCT Int. Appl., 64 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9521175	A1	19950810	WO 1995-US1490	19950202
W: AU, CA, FI, JP, KR, NO				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2182485	AA	19950810	CA 1995-2182485	19950202
AU 9518712	A1	19950821	AU 1995-18712	19950202
AU 691886	B2	19980528		
EP 742789	A1	19961120	EP 1995-910923	19950202
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
JP 09508900	T2	19970909	JP 1995-520799	19950202
EP 1008342	A2	20000614	EP 2000-102434	19950202
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE				
FI 9603045	A	19960801	FI 1996-3045	19960801
NO 9603224	A	19960927	NO 1996-3224	19960801
PRIORITY APPLN. INFO.:			US 1994-190295	19940202
			EP 1995-910923	19950202
			WO 1995-US1490	19950202

OTHER SOURCE(S): MARPAT 124:768

AB Compds. R1Y1CHZ1CH(NY2Y3)CH2Z2 [R1 = straight-chain C8-19 alkyl, alkenyl or alkynyl; Y1 = CH=CH, C|C, CH(OH)CH(OH); Z1 = OH, conversion-inhibiting group; Z2 = conversion-inhibiting group; Y2 = H, Ph, (C1-6 alkyl)-substituted Ph, C1-6 alkyl; Y3 = H, C(O)R2, -S(O)2R2; R2 = straight-chain C1-23 alkyl, alkenyl or alkynyl; when Z2 = amino, R2 = C1-9 or C19-23 aliph. chain] are disclosed, as are liposomes contg. such compds. Methods for treating cancer using the compds. and liposomes of the invention are also disclosed. The effect of e.g. various liposomal ceramide/sphingomyelin formulations on the growth of e.g. HL-60 cells was detd.

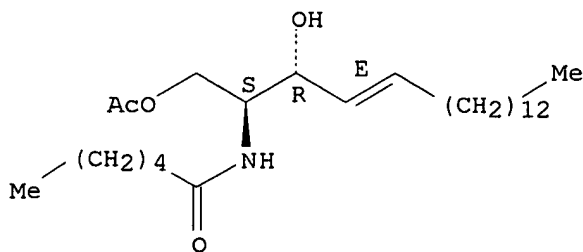
IT 170925-95-8 170925-96-9 170925-97-0
 170925-98-1 170925-99-2 170926-01-9
 170926-08-6 170926-09-7 170926-10-0

RL: BAC (Biological activity or effector, except adverse); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (sphingolipid compds., liposomes contg. them, and methods of use, esp. for cancer therapy)

RN 170925-95-8 CAPLUS

CN Hexanamide, N-[1-[(acetyloxy)methyl]-2-hydroxy-3-heptadecenyl]-, [R-[R*,S*-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
 Double bond geometry as shown.

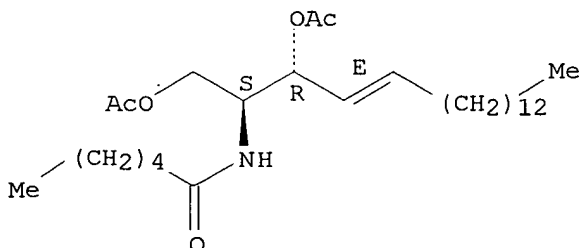


RN 170925-96-9 CAPLUS

Searched by Barb O'Bryen & Toby Port

CN Hexanamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-,
[R-[R*,S*-(E)]]- (9CI) (CA INDEX NAME)

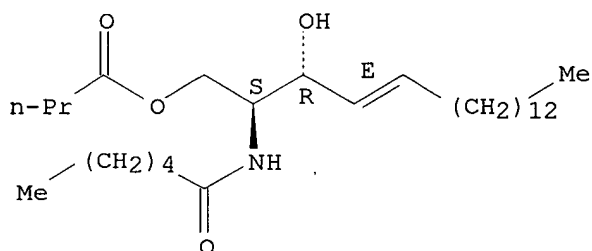
Absolute stereochemistry.
Double bond geometry as shown.



RN 170925-97-0 CAPLUS

CN Butanoic acid, 3-hydroxy-2-[(1-oxohexyl)amino]-4-octadecenyl ester,
[R-[R*,S*-(E)]]- (9CI) (CA INDEX NAME)

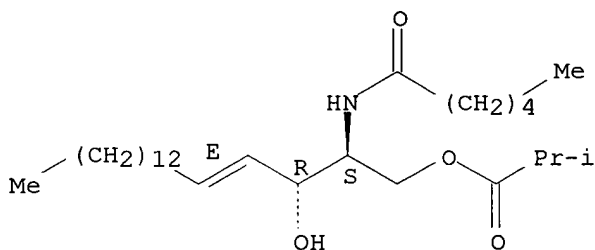
Absolute stereochemistry.
Double bond geometry as shown.



RN 170925-98-1 CAPLUS

CN Propanoic acid, 2-methyl-, 3-hydroxy-2-[(1-oxohexyl)amino]-4-octadecenyl
ester, [R-[R*,S*-(E)]]- (9CI) (CA INDEX NAME)

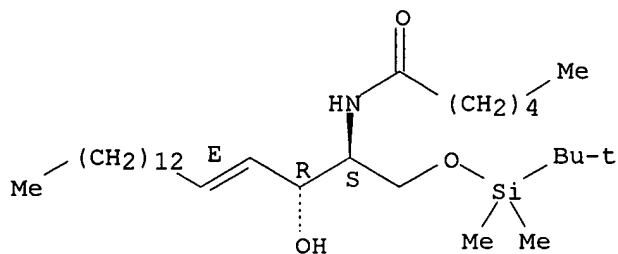
Absolute stereochemistry.
Double bond geometry as shown.



RN 170925-99-2 CAPLUS

CN Hexanamide, N-[1-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-2-hydroxy-3-heptadecenyl]-, [R-[R*,S*-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

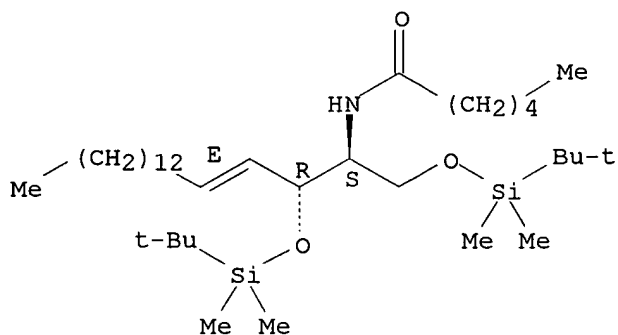


RN 170926-01-9 CAPLUS

CN Hexanamide, N-[2-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-1-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-heptadecenyl]-, [R-[R*,S*-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

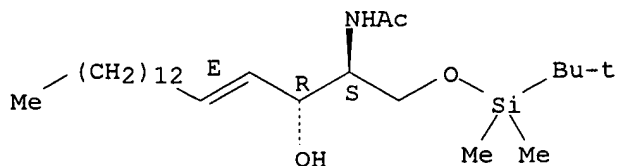


RN 170926-08-6 CAPLUS

CN Acetamide, N-[1-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-2-hydroxy-3-heptadecenyl]-, [R-[R*,S*-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

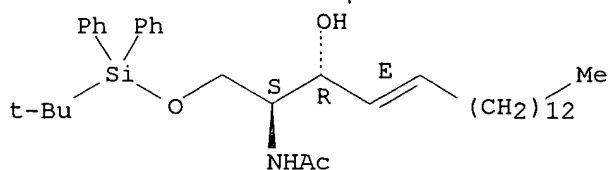


RN 170926-09-7 CAPLUS

CN Acetamide, N-[1-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]methyl]-2-hydroxy-3-heptadecenyl]-, [R-[R*,S*-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

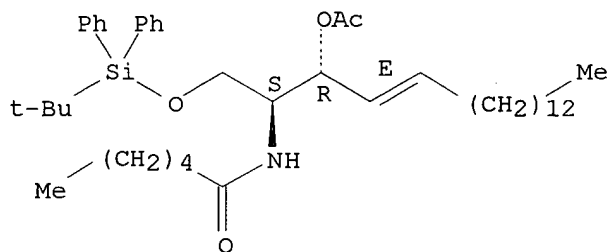


RN 170926-10-0 CAPLUS

CN Hexanamide, N-[2-(acetyloxy)-1-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]methyl]-3-heptadecenyl]-, [R-[R*,S*-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



L32 ANSWER 15 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1995:819842 CAPLUS

DOCUMENT NUMBER: 124:30186

TITLE: Diastereo- and enantioselective synthesis of L-threo- and D-erythro-sphingosine

AUTHOR(S): Enders, Dieter; Whitehouse, Darren L.; Runsink, Jan

CORPORATE SOURCE: Inst. Organische Chemie, Technischen Hochschule, Aachen, D-52074, Germany

SOURCE: Chem.--Eur. J. (1995), 1(6), 382-8

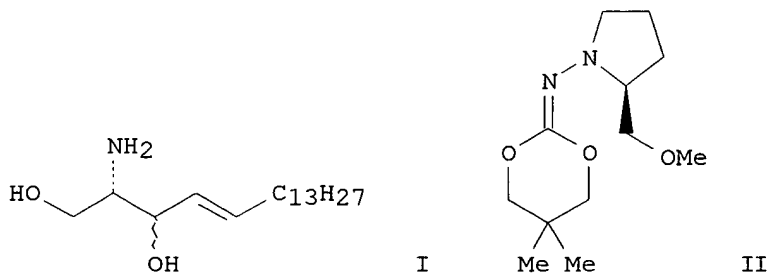
Published in: Angew. Chem., Int. Ed. Engl., 34, 17

CODEN: CEUJED; ISSN: 0947-6539

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB Asym. synthesis of L-threo-sphingosine and its D-erythro isomer I via aldol reaction of the SAMP hydrazone (S)-II with racemic .alpha.-phenylselenylpentadecanal Me(CH2)12(SePh)CHO is reported.

IT 78779-96-1P 116612-39-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
Searched by Barb O'Bryen & Toby Port

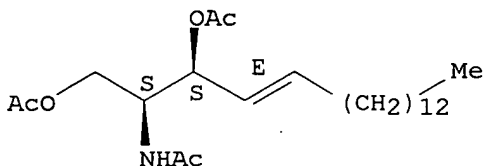
(diastereo- and enantioselective synthesis of L-threo- and D-erythro-sphingosine)

RN 78779-96-1 CAPLUS

CN Acetamide, N-[(1S,2S,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

Double bond geometry as shown.

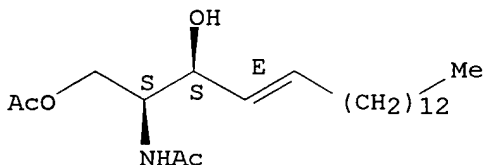


RN 116612-39-6 CAPLUS

CN Acetamide, N-[1-[(acetyloxy)methyl]-2-hydroxy-3-heptadecenyl]-, [S-[R*,R*-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



IT 2482-37-3P

RL: SPN (Synthetic preparation); PREP (Preparation)

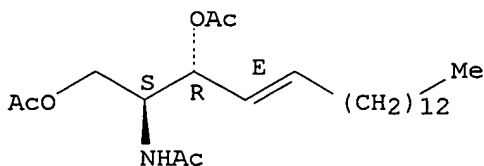
(diastereo- and enantioselective synthesis of L-threo- and D-erythro-sphingosine)

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

Double bond geometry as shown.



L32 ANSWER 16 OF 72 CAPLUS COPYRIGHT 2000 ACS

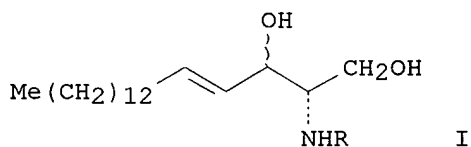
ACCESSION NUMBER: 1995:520214 CAPLUS

DOCUMENT NUMBER: 123:83890

TITLE: Sphingolipid bases. A revisit of the O-methyl derivatives of sphingosine. Isolation and characterization of diacetate derivatives, with revised ¹³C nuclear magnetic resonance assignments for D-erythro-sphingosine

AUTHOR(S): Kisic, Alemka; Tsuda, Mitsuhiro; Kulmacz, Richard J.; Wilson, William K.; Schroepfer, George J., Jr.
Searched by Barb O'Bryen & Toby Port

CORPORATE SOURCE: Dep. Biochemistry, Rice Univ., Houston, TX, 77251, USA
 SOURCE: J. Lipid Res. (1995), 36(4), 787-803
 CODEN: JLPRAW; ISSN: 0022-2275
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB Isolation by medium pressure liq. chromatog. and mol. structure of D-erythro-sphingosine diacetates, e.g. I (R = H, Ac), are reported. Structures were detd. by phys., chromatog., and spectral properties. The 5-O-Me ethers, which were the predominant byproducts of sphingolipid hydrolysis, were easily distinguished from the 3-O-Me ethers by chromatog., and all four isomers could be differentiated by ¹H and ¹³C NMR (NMR) spectroscopy. Resoln. enhancement of the 126-MHz ¹³C NMR spectra of the O-Me ethers and D-erythro-C18-sphingosine I (R = H) afforded distinct signals for nearly all carbon atoms. ¹³C NMR assignments of carbons 7-15 were made from their lanthanide-induced shifts, and revised assignments for olefinic carbons at I (R = H) were established based upon ¹H-¹³C shift correlation expts.

IT 2482-37-3 78779-96-1

RL: PRP (Properties)

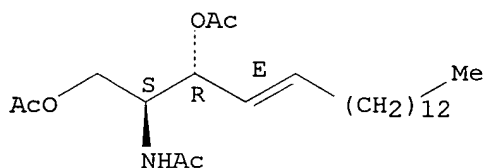
(isolation and mol. structure characterization of D-erythro-sphingosine diacetates)

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

Double bond geometry as shown.

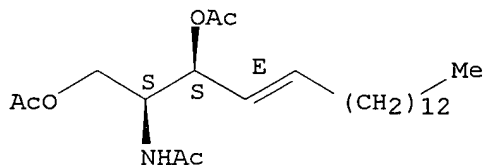


RN 78779-96-1 CAPLUS

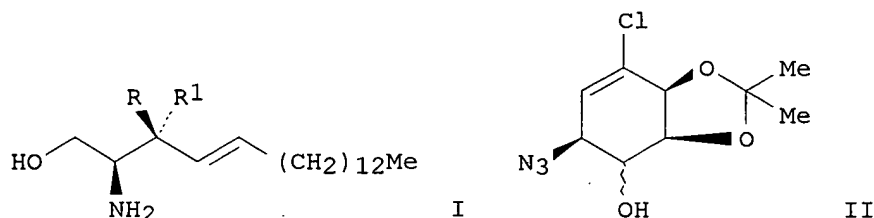
CN Acetamide, N-[(1S,2S,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

Double bond geometry as shown.



L32 ANSWER 17 OF 72 CAPLUS COPYRIGHT 2000 ACS
 ACCESSION NUMBER: 1995:229666 CAPLUS
 DOCUMENT NUMBER: 122:133593
 TITLE: Chemoenzymic Synthesis of D-erythro- and L-threo-C18-Sphingosines
 AUTHOR(S): Hudlicky, Tomas; Nugent, Thomas; Griffith, William
 CORPORATE SOURCE: Department of Chemistry, Virginia Polytechnic Institute and State University, Blacksburg, VA, 24061, USA
 SOURCE: J. Org. Chem. (1994), 59(26), 7944-6
 CODEN: JOCEAH; ISSN: 0022-3263
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB Two sphingosine stereoisomers, the natural isomer I (R = H, R1 = OH) and the L-threo isomer I (R = OH, R1 = H), were prepd. from azido alcs. II via biol. oxidn. of chlorobenzene with toluene dioxygenase from the whole cells of *Pseudomonas putida* 39D.

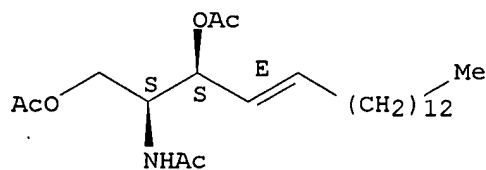
IT 78779-96-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of sphingosine stereoisomers via stereoselective toluene dioxygenase oxidn. of chlorobenzene)

RN 78779-96-1 CAPLUS

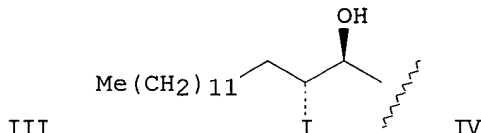
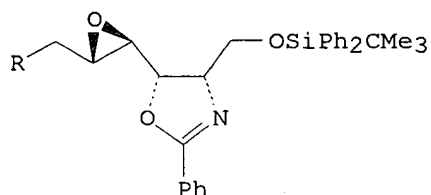
CN Acetamide, N-[(1S,2S,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
 Double bond geometry as shown.



L32 ANSWER 18 OF 72 CAPLUS COPYRIGHT 2000 ACS
 ACCESSION NUMBER: 1994:533751 CAPLUS
 DOCUMENT NUMBER: 121:133751
 TITLE: Regio- and stereocontrolled synthesis of D-erythro-sphingosine and phytosphingosine from D-glucosamine
 AUTHOR(S): Murakami, Teiichi; Minamikawa, Hiroyuki; Hato, Masakatsu
 Searched by Barb O'Bryen & Toby Port

CORPORATE SOURCE: Natl. Inst. Mater. Chem. Res., Tsukuba, 305, Japan
 SOURCE: Tetrahedron Lett. (1994), 35(5), 745-8
 CODEN: TELEAY; ISSN: 0040-4039
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB D-Erythro-sphingosine (I) and phytosphingosine (II) have been efficiently synthesized from D-glucosamine by utilizing its whole carbon skeleton and functional groups. In this synthetic route, regioselective alkylation of the epoxy tosylate III [R = 4-MeC6H4SO3] was achieved with a copper(I)-catalyzed Grignard reagent to give the key intermediate III [R = (CH₂)₁₁Me], which was converted to both I and II via regioselective formation of the iodohydrin IV.

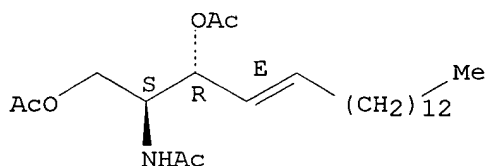
IT 2482-37-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).
 Double bond geometry as shown.



L32 ANSWER 19 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1994:436061 CAPLUS

DOCUMENT NUMBER: 121:36061

TITLE: A Four-Step Diastereoselective Synthesis of
 D-erythro-Sphingosine by an Enantioselective Aldol
 Reaction Using a Titanium Enolate Derived from a
 Chiral Iminoglycinate

AUTHOR(S): Solladie-Cavallo, Arlette; Koessler, Jean L.

CORPORATE SOURCE: Laboratoire de Stereochimie Organometallique,
 E.H.I.C.S., Strasbourg, 67008, Fr.

SOURCE: J. Org. Chem. (1994), 59(11), 3240-2

CODEN: JOCEAH; ISSN: 0022-3263

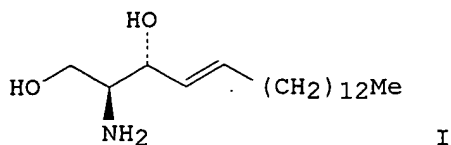
DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 121:36061

GI

Searched by Barb O'Bryen & Toby Port



AB A 4-step synthesis of D-erythro-sphingosine I, with recovery of the chiral auxiliary, is described. The detg. step is a diastereo- and enantioselective aldol reaction using a directly-generated titanium enolate.

IT **2482-37-3P**

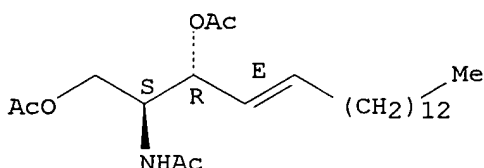
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

Double bond geometry as shown.



L32 ANSWER 20 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1994:226633 CAPLUS

DOCUMENT NUMBER: 120:226633

TITLE: Three glycosphingolipids having the phosphocholine group from the crude drug "Jiryu" (the earthworm, *Pheretima asiatica*)

AUTHOR(S): Noda, Naoki; Tanaka, Ryuichiro; Miyahara, Kazumoto; Kawasaki, Toshio

CORPORATE SOURCE: Fac. Pharm. Sci., Setsunan Univ., Hirakata, 573-01, Japan

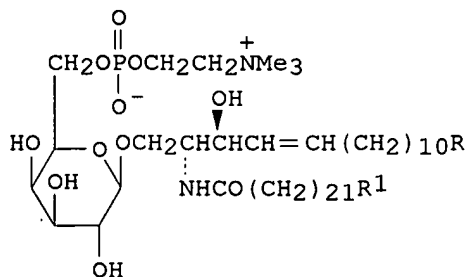
SOURCE: Chem. Pharm. Bull. (1993), 41(10), 1733-7

CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I, R=CHMe₂, R¹=H

II, R=Pr, R¹=H

III, R=Pr, R¹=Et

Searched by Barb O'Bryen & Toby Port

AB Three glycosphingolipids were isolated in the pure state from the crude drug, "Jiryu" (the earthworm, *Pheretima asiatica*). Their structures were detd. as I-III. They are zwitterionic glycosphingolipids having a phosphocholine group attached to the sugar moiety, resembling those obtained from two kinds of marine annelid, and one has a branched long-chain base.

IT **2482-37-3P**

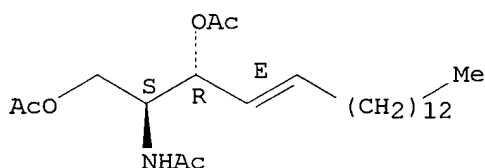
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

Double bond geometry as shown.



L32 ANSWER 21 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1993:427905 CAPLUS

DOCUMENT NUMBER: 119:27905

TITLE: Stereoselective synthesis of D-(+)-erythro- and L-(-)-threo-Sphingosines from carbohydrates

AUTHOR(S): Yadav, J. S.; Vidyanand, D.; Rajagopal, D.

CORPORATE SOURCE: Indian Inst. Chem. Technol., Hyderabad, 500007, India

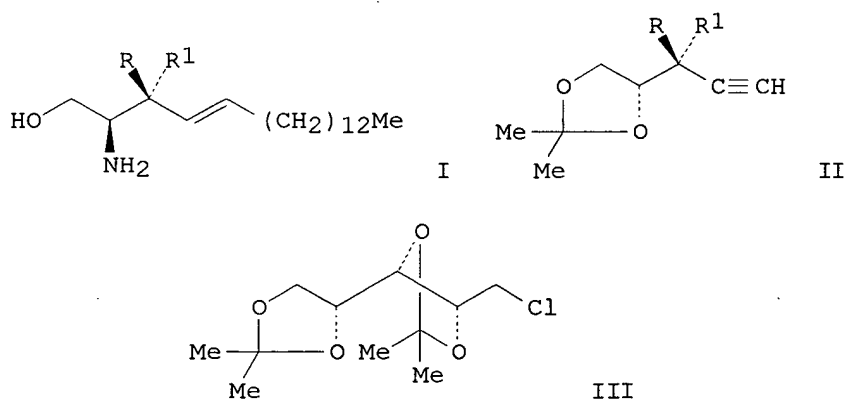
SOURCE: Tetrahedron Lett. (1993), 34(7), 1191-4

CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB Stereocontrolled syntheses of D-(+)-erythro and L-(-)-threo-sphingosines I (R = H, R1 = HO; R = HO, R1 = H resp) are described starting from D-xylose and D-arabinose resp. through acetylenic intermediates II (same R, R1),
Searched by Barb O'Bryen & Toby Port

obtained by base induced double elimination of the .beta.-alkoxy chlorides, e.g. III.

IT **78779-96-1P**

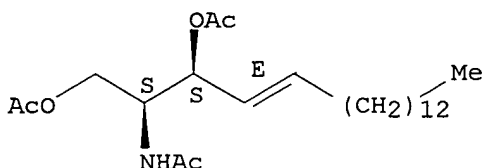
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 78779-96-1 CAPLUS

CN Acetamide, N-[(1S,2S,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

Double bond geometry as shown.



L32 ANSWER 22 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1993:45757 CAPLUS

DOCUMENT NUMBER: 118:45757

TITLE: Amino alcohol derivatives as membrane penetration enhancers

INVENTOR(S): Rajadhyaksha, Vithal J.

PATENT ASSIGNEE(S): USA

SOURCE: PCT Int. Appl., 43 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

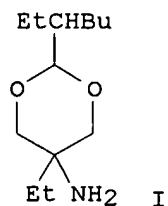
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9216236	A1	19921001	WO 1992-US2219	19920319
W: AU, CA, JP				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, MC, NL, SE				
CA 2106483	AA	19920920	CA 1992-2106483	19920319
AU 9217451	A1	19921021	AU 1992-17451	19920319
AU 664178	B2	19951109		
EP 576605	A1	19940105	EP 1992-910289	19920319
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, MC, NL, SE				
JP 06509559	T2	19941027	JP 1992-509964	19920319
US 5482965	A	19960109	US 1993-115772	19930903
PRIORITY APPLN. INFO.:			US 1991-672020	19910319
			WO 1992-US2219	19920319

OTHER SOURCE(S): MARPAT 118:45757

GI



AB Amino alcs., including dioxane derivs., are prepd. as penetration enhancers for topical pharmaceuticals. I was prepd. from 2-ethylhexanal and 5-nitro-1,3-dioxane and redn. of the product. An analgesic gel was prepd. contg. Carbopol 941 1.5, diclofenac Na 1, 2-propanol 35, diisopropanolamine 1.8, diisopropyl adipate 5, I 2, and water 53.7%.

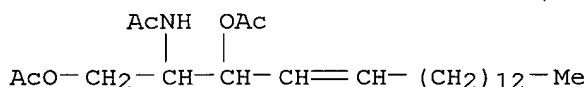
IT 96579-26-9 145277-15-2

RL: BIOL (Biological study)

(penetration enhancer, for topical pharmaceuticals)

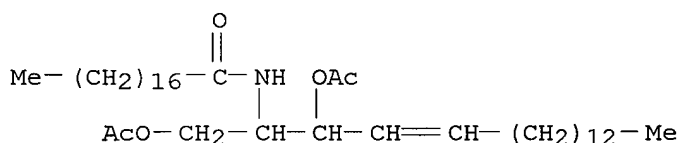
RN 96579-26-9 CAPLUS

CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI)
(CA INDEX NAME)



RN 145277-15-2 CAPLUS

CN Octadecanamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)



L32 ANSWER 23 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1992:571846 CAPLUS

DOCUMENT NUMBER: 117:171846

TITLE: Sphingolipids and glycerolipids. II. Syntheses of two pairs of enantiomeric C18-sphingosines and a palmitoyl analog of Gaucher spleen glucocerebroside
AUTHOR(S): Shibuya, Hirotaka; Kawashima, Keiko; Narita, Norihiko; Ikeda, Masahiko; Kitagawa, Isao

CORPORATE SOURCE: Fac. Pharm. Sci., Osaka Univ., Suita, 565, Japan

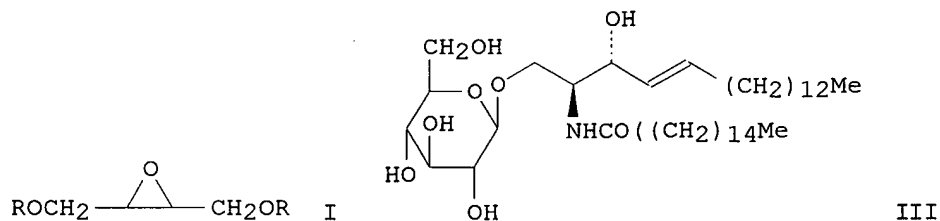
SOURCE: Chem. Pharm. Bull. (1992), 40(5), 1154-65

CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB Sixteen chiral C4 epoxides I (R = 4-MeOC6H4CPh2, PhCH2, MeOCH2, Searched by Barb O'Bryen & Toby Port

Me₃CSiMe₂), which are synthons for complex lipids, have been prepd. from (2Z)-2-butene-1,4-diol by employing a Sharpless asym. epoxidn. By using I as starting compds., two pairs of enantiomeric C18 sphingosines (E)-HOCH₂CH(NH₂)CH(OH)CH:CH(CH₂)₁₂Me (II) have been synthesized via a regioselective ring-opening of the epoxide ring with azide anion followed by redn. of the azide group to an amino group and a Wittig reaction. Furthermore, D-erythro-II has been converted to the palmitoyl analog III of Gaucher spleen glucocerebroside through a reaction pathway including successive condensations with palmitic acid and D-glucose.

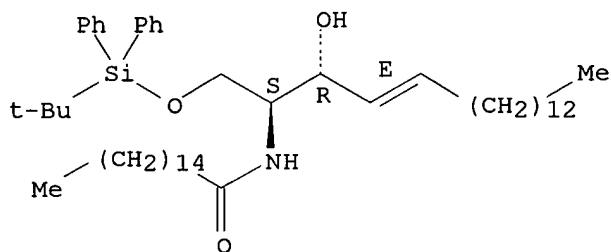
IT 143517-08-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and benzylation of)

RN 143517-08-2 CAPLUS

CN Hexadecanamide, N-[(1S,2R,3E)-1-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]methyl]-2-hydroxy-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



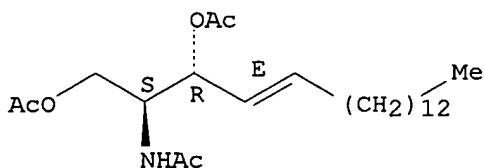
IT 2482-37-3P 128387-02-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and deblocking of)

RN 2482-37-3 CAPLUS

CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

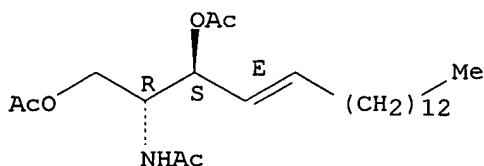
Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.



RN 128387-02-0 CAPLUS

CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-, [S-[R*,S*-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



Searched by Barb O'Bryen & Toby Port

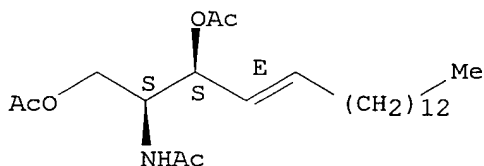
IT 78779-96-1P 128387-01-9P 128387-05-3P
143615-68-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 78779-96-1 CAPLUS

CN Acetamide, N-[(1S,2S,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

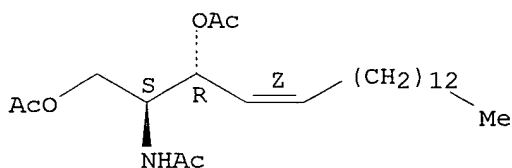
Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



RN 128387-01-9 CAPLUS

CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-, [R-[R*,S*-(Z)]]- (9CI) (CA INDEX NAME)

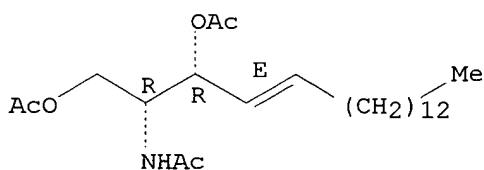
Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



RN 128387-05-3 CAPLUS

CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-, [R-[R*,R*-(E)]]- (9CI) (CA INDEX NAME)

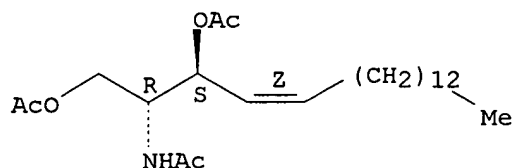
Absolute stereochemistry.
Double bond geometry as shown.



RN 143615-68-3 CAPLUS

CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-, [S-[R*,S*-(Z)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L32 ANSWER 24 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1992:571057 CAPLUS

DOCUMENT NUMBER: 117:171057

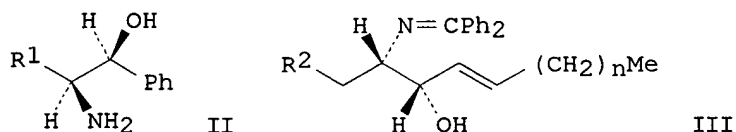
TITLE: Aluminoxy acetals from .alpha.-amino esters:
chirality transfer via sequential addition of hydride
and C-nucleophiles. 2-Amino alcohols and sphingosines
AUTHOR(S): Polt, Robin; Peterson, Matt A.; DeYoung, Lynn
CORPORATE SOURCE: Dep. Chem., Univ. Arizona, Tucson, AZ, 85721, USA
SOURCE: J. Org. Chem. (1992), 57(20), 5469-80
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 117:171057

GI



AB The reaction of .alpha.-imino esters with aluminum hydrides to produce acetal-like intermediates and subsequent reaction with carbon nucleophiles has been studied. Treatment of optically pure imine-protected amino esters with *i*-Bu₂AlH or *i*-Bu₂AlH.cntdot.*i*-Bu₃Al, followed by RMgX or RLi provided threo-2-amino alcs. in high yield (73-85%) and excellent syn stereoselectivity (8:1 to >20:1, threo or threo-like product preferred). Use of nonpolar solvents (CH₂Cl₂-hexane) provided the highest stereoselectivities. Use of the less-reactive *i*-Bu₂AlH.cntdot.*i*-Bu₃Al complex lowered the amt. of undesired primary alc. products obsd. Thermally labile aluminoxy acetal intermediates were obsd. by ¹H NMR and were trapped with N-(trimethylsilyl)imidazole to produce relatively stable monosilyl acetals (mixed acetals). Alanine-derived Schiff bases (S)-Ph₂C:NCHMeCO₂R (I; R = Me, Et, CH₂Ph, CHPh₂, CMe₃) showed a correlation between the steric bulk of the ester and threo selectivity. The presence of THF reduced this correlation, suggesting the C-nucleophile addn. involves a Lewis acid-assisted S_N2-like displacement of the aluminoxy acetal or displacement of a tight-ion pair. In addn. to the synthesis of optically pure aryethanolamines II (R₁ = H, Me, CH₂Ph, CH₂OSiMe₂CMe₃) from representative amino acids, threo-sphingosines III (R₂ = OSiMe₂CMe₃, n = 3, 4, 7, 12) were synthesized from L-serine-derived Schiff base (S)-Ph₂C:NCH(CH₂OSiMe₂CMe₃)CO₂Me, and 1-deoxy-threo-sphingosines III (R₂ = H, n = same) were synthesized from I (R = Me) in a similar fashion. Exptl. details are provided.

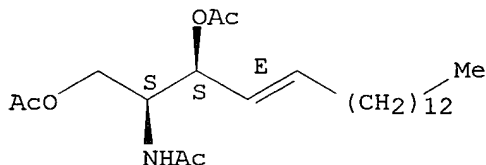
IT 78779-96-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

Searched by Barb O'Bryen & Toby Port

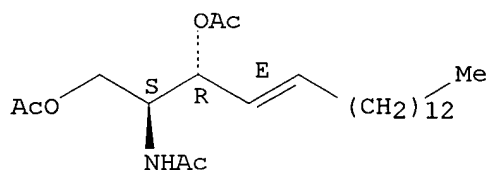
RN 78779-96-1 CAPLUS
 CN Acetamide, N-[(1S,2S,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
 Double bond geometry as shown.



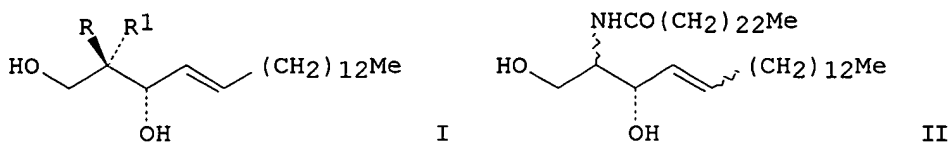
L32 ANSWER 25 OF 72 CAPLUS COPYRIGHT 2000 ACS
 ACCESSION NUMBER: 1992:59850 CAPLUS
 DOCUMENT NUMBER: 116:59850
 TITLE: The synthesis of glycosphingolipids: I. The synthesis of lactosylceramide and lactosylsphingenine and a short synthesis of triacetyl-D-erythro-sphingosine. II. The synthesis of the Lex family of glycosphingolipids
 AUTHOR(S): Caulfield, Thomas Joseph
 CORPORATE SOURCE: Univ. Pennsylvania, Philadelphia, PA, USA
 SOURCE: (1991) 358 pp. Avail.: Univ. Microfilms Int., Order No. DA9125609
 From: Diss. Abstr. Int. B 1991, 52(3), 1432
 DOCUMENT TYPE: Dissertation
 LANGUAGE: English
 AB Unavailable
 IT **2482-37-3P**
 RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)
 RN 2482-37-3 CAPLUS
 CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).
 Double bond geometry as shown.



L32 ANSWER 26 OF 72 CAPLUS COPYRIGHT 2000 ACS
 ACCESSION NUMBER: 1992:41172 CAPLUS
 DOCUMENT NUMBER: 116:41172
 TITLE: Enantiospecific syntheses of sphingosine and ceramide stereoisomers with 3S configuration from D-glucose
 AUTHOR(S): Fujita, Shuji; Sugimoto, Mamoru; Tomita, Kenkichi; Nakahara, Yoshiaki; Ogawa, Tomoya
 CORPORATE SOURCE: MECT Corp., Saitama, 359, Japan
 SOURCE: Agric. Biol. Chem. (1991), 55(10), 2561-9
 CODEN: ABCHA6; ISSN: 0002-1369
 DOCUMENT TYPE: Journal
 Searched by Barb O'Bryen & Toby Port

LANGUAGE: English
GI



AB Starting from D-glucose, 2-amino-4-octadecene-1,3-diols I (R = H, R1 = NH₂; R = NH₂, R1 = H) and 4 stereoisomers of tetracosanoylsphingene II were prepd.

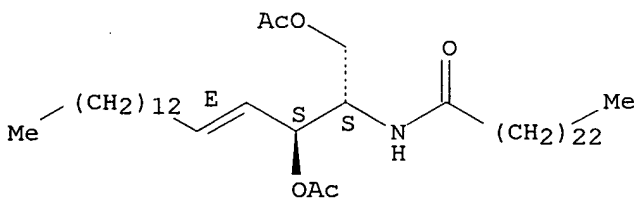
IT **121468-17-5P 121468-18-6P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 121468-17-5 CAPLUS

CN Tetracosanamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-, [S-[R*,R*-(E)]]- (9CI) (CA INDEX NAME)

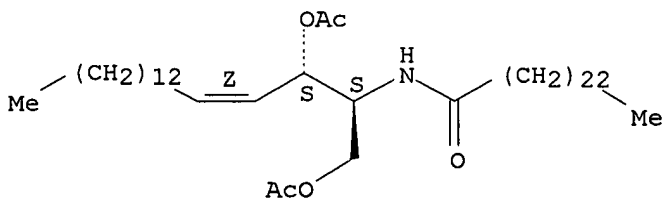
Absolute stereochemistry.
Double bond geometry as shown.



RN 121468-18-6 CAPLUS

CN Tetracosanamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-, [S-[R*,R*-(Z)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L32 ANSWER 27 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1991:680423 CAPLUS

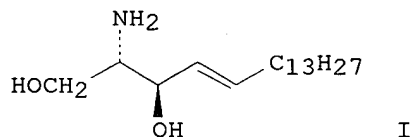
DOCUMENT NUMBER: 115:280423

TITLE: A convenient stereoselective synthesis of
D-erythro-C18-sphingosine from galactal

AUTHOR(S): Hirata, Norihiko; Yamagiwa, Yoshiro; Kamikawa, Tadao
CORPORATE SOURCE: Fac. Sci. Technol., Kinki Univ., Higashi-Osaka, 577,
Japan

SOURCE: J. Chem. Soc., Perkin Trans. 1 (1991), (9), 2279-80
Searched by Barb O'Bryen & Toby Port

DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 115:280423
 GI



AB The highly efficient stereoselective synthesis of title sphingosine I from 3,4,6-tribenzyloxygalactal in 9 steps and 26% overall yield, via 4,6-tribenzyloxy-5-hydroxyhexenal, is described.

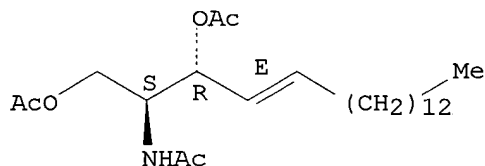
IT 2482-37-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).
 Double bond geometry as shown.



L32 ANSWER 28 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1991:626541 CAPLUS

DOCUMENT NUMBER: 115:226541

TITLE: Interaction of cholesterol with synthetic sphingomyelin derivatives in mixed monolayers

AUTHOR(S): Gronberg, Lotte; Ruan, Zhongshi; Bittman, Robert; Slotte, J. Peter

CORPORATE SOURCE: Dep. Biochem. Pharm., Abo Akad. Univ., Turku, SF-20500, Finland

SOURCE: Biochemistry (1991), 30(44), 10746-54

CODEN: BICHAW; ISSN: 0006-2960

DOCUMENT TYPE: Journal

LANGUAGE: English

AB To study the structural requirements of the mol. interactions between cholesterol and sphingomyelins in model membranes, sphingomyelin derivs. were synthesized in which (a) the 3-hydroxy group was replaced with a hydrogen atom or with a methoxy, ethoxy, or tetrahydropyranyloxy group, (b) the N-acyl chain length was varied, and (c) the N-acyl chain length contained an .alpha.-hydroxy group. The chem. syntheses of these derivs. from DL-erythro-sphingosine are reported. The properties of these sphingomyelin derivs. were examd. in monolayer membranes at the air/water interface. The mean mol. area of the pure N-stearoylsphingomyelin derivs. was detd., and the effects of cholesterol on the condensation of sphingomyelin packing in the monolayer were recorded. It was obsd. that replacement of the 3-hydroxy group of sphingomyelin with a hydrogen atom

Searched by Barb O'Bryen & Toby Port

or its substitution with a methoxy or ethoxy group did not affect the ability of cholesterol to condense the mol. packing in monolayers. Even when a bulky tetrahydropyranyloxy group was introduced at the 3-hydroxy position of egg sphingomyelin, cholesterol was still able to condense the mol. packing of this deriv. The condensing effect of cholesterol on derivs. of N-stearoylsphingomyelins was significantly larger than the comparable effect obsd. with 1,2-distearoyl-sn-glycero-3-phosphocholine or 1,2-dipalmitoyl-sn-glycero-3-phosphocholine. Results with 3-hydroxysphingomyelins having differing N-acyl chain lengths (i.e., N-stearoyl, N-myristoyl, and N-lauroyl), and with 3-hydroxy-N-(.alpha.-hydroxypalmitoyl)sphingomyelin also indicated that cholesterol was able to induce condensation of the mol. packing. Another measure of the mol. packing in monolayers is the cholesterol oxidase susceptibility of cholesterol embedded in sphingomyelin-contg. monolayers. The rate of enzyme-catalyzed cholesterol oxidn. in monolayers contg. 3-hydroxy-substituted N-stearoylsphingomyelins was about 30% lower than the comparable maximal rate measured in a monolayer of dipalmitoylphosphatidylcholine at the same surface pressure. Substitution of a hydroxy group at the .alpha. position of the amide chain of sphingomyelin did not perturb the projection of the sterol's 3.beta.-hydroxy group toward the lipid/water interface. Cholesterol was, however, oxidized about 50% faster in monolayers contg. 3-hydroxysphingomyelins with shorter acyl chains (i.e., N-lauroyl and N-myristoyl) than with a N-stearoyl chain, the rate being similar to that obsd. in a dipalmitoylphosphatidylcholine/cholesterol mixed monolayer. It is concluded that the 3-hydroxy group of sphingomyelin is not required for the efficient interaction between cholesterol and sphingomyelin in monolayer membranes. Furthermore, shortening the N-acyl group of sphingomyelin by 4 to 6 methylene groups had only a marginal effect on this interaction in monolayers.

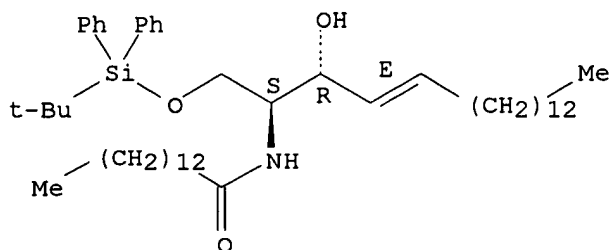
IT 136794-89-3P 136794-91-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and conversion to tetrahydropyranyl deriv.)

RN 136794-89-3 CAPLUS

CN Tetradecanamide, N-[1-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]methyl]-2-hydroxy-3-heptadecenyl]-, [R*,S*-(E)]- (9CI) (CA INDEX NAME)

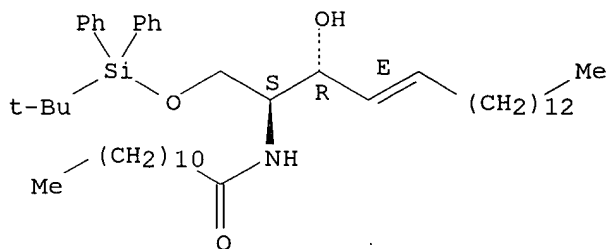
Relative stereochemistry.
Double bond geometry as shown.



RN 136794-91-7 CAPLUS

CN Dodecanamide, N-[1-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]methyl]-2-hydroxy-3-heptadecenyl]-, [R*,S*-(E)]- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



L32 ANSWER 29 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1991:470908 CAPLUS

DOCUMENT NUMBER: 115:70908

TITLE: Total synthesis of chiral 2-amino-1,3-diols

INVENTOR(S): Illig, Carl R.; Weis, Alexander L.

PATENT ASSIGNEE(S): Eastman Kodak Co., USA

SOURCE: U.S., 9 pp.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5012000	A	19910430	US 1989-428799	19891030

OTHER SOURCE(S): CASREACT 115:70908

AB D-erythro-Sphingosine was prepd. in a 4 step synthesis from (S)-3-(chloroacetyl)-4-benzyl-2-oxazolidinone by sequential aldol condensation with trans-2-hexadecenal, azide substitution reaction, NaBH₄ redn. and azide redn. with HS(CH₂)₃SH and Et₃N.

IT 2482-37-3P

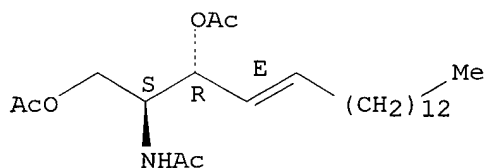
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetoxymethyl)-1-[(acetoxymethyl)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

Double bond geometry as shown.



L32 ANSWER 30 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1991:466885 CAPLUS

DOCUMENT NUMBER: 115:66885

TITLE: Interaction of cholesterol with sphingomyelin in bilayer membranes: evidence that the hydroxy group of sphingomyelin does not modulate the rate of cholesterol exchange between vesicles

AUTHOR(S): Kan, Chu Cheng; Ruan, Zhong Shi; Bittman, Robert
Searched by Barb O'Bryen & Toby Port

CORPORATE SOURCE: Queens Coll., City Univ. New York, Flushing, NY,
11367, USA
SOURCE: Biochemistry (1991), 30(31), 7759-66
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Cholesterol undergoes exchange between membranes contg. sphingomyelin at a much slower rate than between membranes lacking sphingomyelin. To investigate the role of the hydroxy group at the 3-position of sphingomyelin in the interaction between sphingomyelin and cholesterol, the rates of [4-¹⁴C]cholesterol exchange were measured between unilamellar vesicles prep'd. with N-stearoylsphingomyelin or with synthetic analogs in which the hydroxy group is replaced with an O-alkyl group or with hydrogen. Vesicles prep'd. from 3-deoxy- and 3-O-methyl-N-stearoylsphingomyelin had the same rate of [¹⁴C]cholesterol desorption. The half-times for exchange from vesicles prep'd. with 3-O-methyl- and 3-deoxy-N-stearoylsphingomyelins and 10 mol % of cholesterol were only slightly faster (a factor of only 1.5) than that found from vesicles prep'd. from N-stearoylsphingomyelin and 10 mol % cholesterol. The rate of cholesterol desorption from vesicles could be accelerated by prepg. vesicles from bulky 3-O-alkyl analogs of sphingomyelin. Vesicles contg. 3-O-ethyl-N-stearoylsphingomyelin and 3-O-tetrahydropyranyl egg sphingomyelin gave rate enhancements of .apprx.14 and 35, compared with the rates obsd. in vesicles made from N-stearoyl- and egg sphingomyelin, resp. These data indicate that insertion of sterically bulky groups at the 3-position of sphingomyelin (such as ethoxy and tetrahydropyranyloxy) in place of hydroxy interferes markedly with the mol. packing of cholesterol and sphingomyelin in bilayer membranes; however, the hydroxy group of sphingomyelin is not crit. for the strong interaction of cholesterol with sphingomyelin. These results suggest that van der Waals interactions are more important than hydrogen-bonding interactions involving the hydroxy group in contributing to tight lateral packing of cholesterol with sphingomyelin.

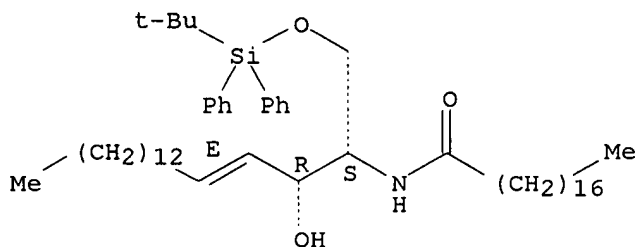
IT 134654-02-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction with Me iodide)

RN 134654-02-7 CAPLUS

CN Octadecanamide, N-[1-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]methyl]-2-hydroxy-3-heptadecenyl]-, [R*,S*-(E)]- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



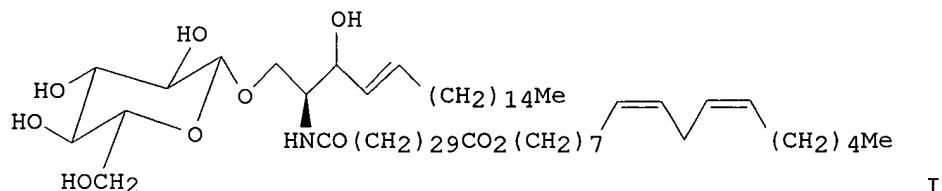
L32 ANSWER 31 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1991:429780 CAPLUS

DOCUMENT NUMBER: 115:29780

TITLE: Synthesis of sphingosine relatives. X. Synthesis of (2S, 3R, 4E)-1-O-(.beta.-D-glucopyranosyl)-N-[30'-(linoleoyloxy)triacontanoyl]-4-icosasphingenine, a new esterified cerebroside isolated from human and pig
Searched by Barb O'Bryen & Toby Port

epidermis
 AUTHOR(S): Mori, Kenji; Matsuda, Hiroyuki
 CORPORATE SOURCE: Dep. Agric. Chem., Univ. Tokyo, Tokyo, 113, Japan
 SOURCE: Liebig's Ann. Chem. (1991), (6), 529-35
 CODEN: LACHDL; ISSN: 0170-2041
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



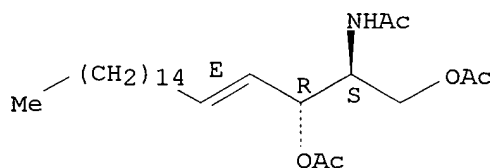
AB Glucopyranosylcosasphingenine I was synthesized from D-glucose, L-serine, 15-pentadecanolide, and linoleic acid. The high-field ^1H NMR spectrum of I was identical with that of the esterified cerebroside isolated from human and pig epidermis.

IT **25494-35-3P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

RN 25494-35-3 CAPLUS

CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-nonadecenyl]-, [R-[R*,S*-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
 Double bond geometry as shown.



L32 ANSWER 32 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1991:229262 CAPLUS

DOCUMENT NUMBER: 114:229262

TITLE: Asymmetric synthesis via heterocyclic intermediates.

43. Asymmetric synthesis of D-erythro-sphingosine

Groth, Ulrich; Schoellkopf, Ulrich; Tiller, Thomas

CORPORATE SOURCE: Inst. Org. Chem., Univ. Goettingen, Goettingen,

SOURCE: D-3400, Fed. Rep. Ger.

Tetrahedron (1991), 47(16-17), 2835-42

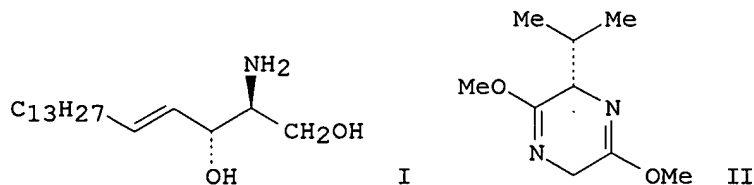
CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 114:229262

GI



AB Title compd. I is a building block of cerebrosides and glycosphingolipids and was synthesized in 5 steps via an asym. aldol addn. of the inhibited bislactim ether of II to (2E)-hexadecenal in an overall yield of 21 %.

IT 2482-37-3P

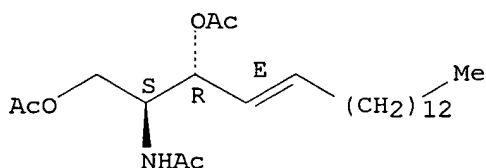
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

Double bond geometry as shown.



L32 ANSWER 33 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1991:207692 CAPLUS

DOCUMENT NUMBER: 114:207692

TITLE: Preparation of unnatural sialosylceramides

INVENTOR(S): Fujita, Hideji; Sugimoto, Mamoru; Ito, Masayoshi;
Ogawa, Tomoya

PATENT ASSIGNEE(S): Mekuto K. K., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 16 pp.

CODEN: JKXXAF

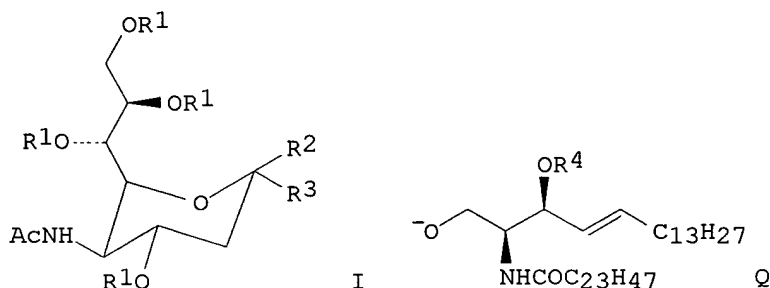
DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 02202895	A2	19900810	JP 1989-23290	19890201
OTHER SOURCE(S): MARPAT 114:207692				
GI				



AB The title compds. [I; R1 = acyl, H; R2, R3 = Q, CO₂R₅; R4 = H, Bz; provided that R2 and R3 may not be simultaneously the same; R5 = alkyl, alk. metal], useful for studying animal cell proliferation (no data), were prepd. via condensation of the appropriate sugar acid derivs. with ceramides HQ. A mixt. of I [R1 = Ac, R2 = Cl, R3 = CO₂Me], HQ [R4 = Bz] (prepn. given), Hg(CN)₂, HgBr₂, mol. sieve 4A, and CHCl₃ was heated in an oil bath at 50.degree. for 2 h gave I [R1 = Ac, R2 = CO₂Me, R3 = Q, R4 = Bz].

IT **121468-17-5P 121468-18-6P**

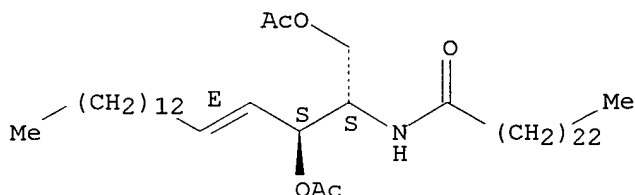
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as intermediate for unnatural sialosylceramides)

RN 121468-17-5 CAPLUS

CN Tetracosanamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-, [S-[R*,R*-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

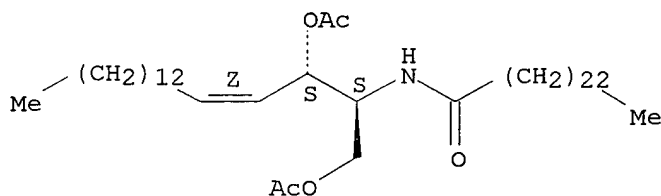


RN 121468-18-6 CAPLUS

CN Tetracosanamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-, [S-[R*,R*-(Z)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



L32 ANSWER 34 OF 72 CAPLUS COPYRIGHT 2000 ACS

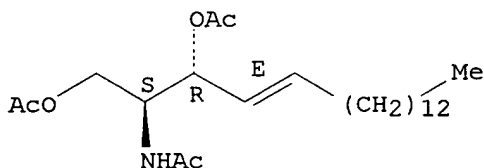
ACCESSION NUMBER: 1991:161128 CAPLUS

DOCUMENT NUMBER: 114:161128

TITLE: Cerebrosides of frog brain. Structure of the ceramide
Searched by Barb O'Bryen & Toby Port

part of the cerebrosides
 AUTHOR(S): Munesada, Kiyotaka; Yuasa, Masatoshi; Suga, Takayuki
 CORPORATE SOURCE: Fac. Sci., Hiroshima Univ., Hiroshima, 730, Japan
 SOURCE: J. Chem. Soc., Perkin Trans. 1 (1991), (1), 189-94
 CODEN: JCPRB4; ISSN: 0300-922X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Twelve cerebrosides were isolated from the brain tissues of the bullfrog (Bana catesbeiana) and were characterized as 1-o-.beta.-D-galactopyranosyl ceramides. On the basis of chem. and spectral evidence, the ceramide parts of six of them were found to be composed of a sphingosine as a long-chain base and six fatty acids consisting of C18:0, C22:1, and C24:1 acids and their 2-hydroxy derivs. The ceramide parts of the others were found to be composed of a dihydroxysphingosine and the six fatty acids. The configurations at C-2 and C-3 of the two long-chain bases were detd. to be S and R, resp. A different distribution of the cerebrosides was seen among the hemisphere, diencephalon and mixed tissue from the optic lobe, cerebellum and medulla oblongata of the brain.
 IT **2482-37-3P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 RN 2482-37-3 CAPLUS
 CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

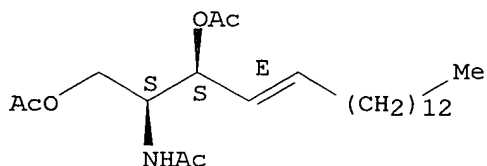
Absolute stereochemistry. Rotation (-).
 Double bond geometry as shown.



L32 ANSWER 35 OF 72 CAPLUS COPYRIGHT 2000 ACS
 ACCESSION NUMBER: 1991:120954 CAPLUS
 DOCUMENT NUMBER: 114:120954
 TITLE: Asymmetric aldol reaction catalyzed by chiral complexes
 AUTHOR(S): Hayashi, Tamio; Ito, Yoshihiko
 CORPORATE SOURCE: Grad. Sch. Pharm. Sci., Hokkaido Univ., Sapporo, 060, Japan
 SOURCE: Yukagaku (1990), 39(10), 846-51
 CODEN: YKGKAM; ISSN: 0513-398X
 DOCUMENT TYPE: Journal
 LANGUAGE: Japanese
 OTHER SOURCE(S): CASREACT 114:120954
 AB Asym. aldol reactions of .alpha.-isocyano carboxylates with aldehydes were catalyzed by gold(I) complexes with a chiral ferrocenylphosphine ligand contg. a [(dialkylamino)ethyl]amino group on the ferrocene side chain. Optically active (up to 98% ee) 5-alkyl-trans-4-(methoxycarbonyl)-2-oxazolines were obtained with high enantio- and diastereoselectivity in quant. yield. The optically active oxazolines were readily converted to .beta.-hydroxy-.alpha.-amino acids and their derivs.
 IT **78779-96-1P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 RN 78779-96-1 CAPLUS
 CN Acetamide, N-[(1S,2S,3E)-2-(acetvloxv)-1-[(acetvloxv)methyl]-3-
 Searched by Barb O'Bryen & Toby Port

heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



L32 ANSWER 36 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1990:531846 CAPLUS

DOCUMENT NUMBER: 113:131846

TITLE: Synthesis of two pairs of enantiomeric
C18-sphingosines

AUTHOR(S): Shibuya, Hiroataka; Kawashima, Keiko; Ikeda, Masahiko;
Kitagawa, Isao

CORPORATE SOURCE: Fac. Pharm. Sci., Osaka Univ., Suita, 565, Japan

SOURCE: Tetrahedron Lett. (1989), 30(51), 7205-8

CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 113:131846

AB D-erythro-, L-erythro-, D-threo-, And L-threo-(E)-
HOCH₂CH(NH₂)CH(OH)CH:CH(CH₂)₁₂Me have been synthesized from
Z-butene-1,4-diol utilizing Sharpless asym. epoxidn. and a regiospecific
ring-opening reaction of the resulting C4 chiral epoxide with an azide
anion.

IT **2482-37-3P 128387-02-0P**

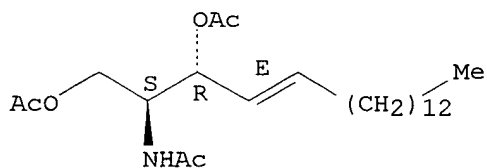
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and deacetylation of)

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-
heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

Double bond geometry as shown.

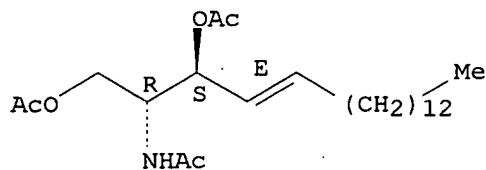


RN 128387-02-0 CAPLUS

CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-,
[S-[R*,S*-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



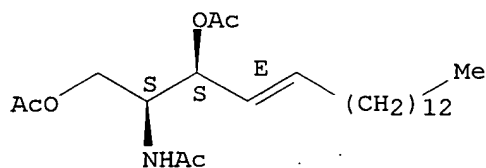
IT 78779-96-1P 128387-01-9P 128387-05-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 78779-96-1 CAPLUS

CN Acetamide, N-[(1S,2S,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

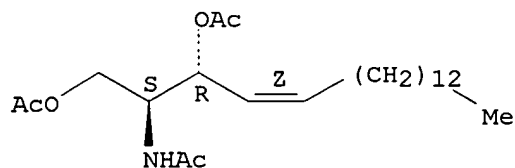
Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



RN 128387-01-9 CAPLUS

CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-, [R-[R*,S*-(Z)]]- (9CI) (CA INDEX NAME)

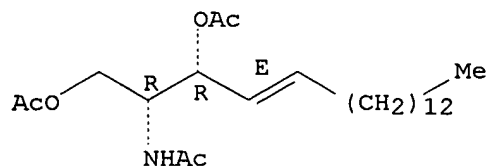
Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



RN 128387-05-3 CAPLUS

CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-, [R-[R*,R*-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L32 ANSWER 37 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1990:497937 CAPLUS

DOCUMENT NUMBER: 113:97937

TITLE: An efficient, stereoselective synthesis of 4-E- and
Searched by Barb O'Bryen & Toby Port

4-Z-D-erythro-sphingene and related compounds from
2-amino-2-deoxy-D-glucose
AUTHOR(S): Sugawara, Tamio; Narisada, Masayuki
CORPORATE SOURCE: Res. Lab., Shionogi and Co., Ltd., Osaka, 553, Japan
SOURCE: Carbohydr. Res. (1989), 194, 125-38
CODEN: CRBRAT; ISSN: 0008-6215

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 113:97937

AB Efficient, stereoselective synthesis of 4-E- and 4-Z-D-erythro-sphingenes having C16, C18, and C20 carbon-chains was achieved in 13 steps, starting from allyl 2-benzyloxycarbonylamino-2-deoxy-.alpha.-D-glucopyranoside. 2-Amino-1,6-di-O-tert-butyldiphenylsilyl-2-N-3-O-carbonyl-2-deoxy-D-allitol was used as the key intermediate.

IT 2482-37-3P 25494-35-3P 128387-01-9P
128745-57-3P

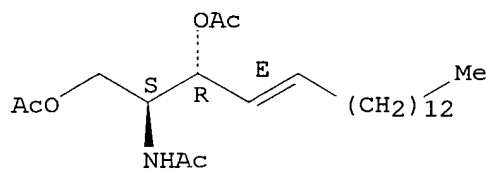
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

Double bond geometry as shown.

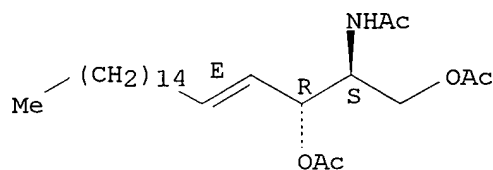


RN 25494-35-3 CAPLUS

CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-nonadecenyl]-, [R-[R*,S*-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

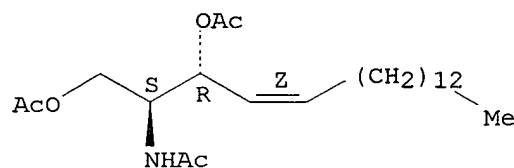


RN 128387-01-9 CAPLUS

CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-, [R-[R*,S*-(Z)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

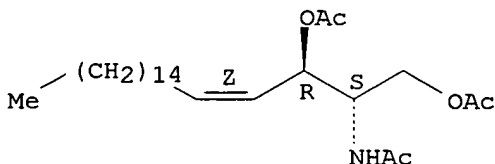
Double bond geometry as shown.



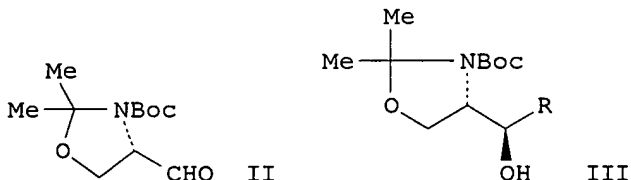
Searched by Barb O'Bryen & Toby Port

RN 128745-57-3 CAPLUS
 CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-nonadecenyl]-,
 [R-[R*,S*-(Z)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
 Double bond geometry as shown.



L32 ANSWER 38 OF 72 CAPLUS COPYRIGHT 2000 ACS
 ACCESSION NUMBER: 1990:119279 CAPLUS
 DOCUMENT NUMBER: 112:119279
 TITLE: Stereochemistry associated with the addition of
 2-(trimethylsilyl)thiazole to differentially protected
 .alpha.-amino aldehydes. Applications toward the
 synthesis of amino sugars and sphingosines
 AUTHOR(S): Dondoni, Alessandro; Fantin, Giancarlo; Fogagnolo,
 Marco; Pedrini, Paola
 CORPORATE SOURCE: Dip. Chim., Univ. Ferrara, Ferrara, Italy
 SOURCE: J. Org. Chem. (1990), 55(5), 1439-46
 CODEN: JOCEAH; ISSN: 0022-3263
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 112:119279
 GI



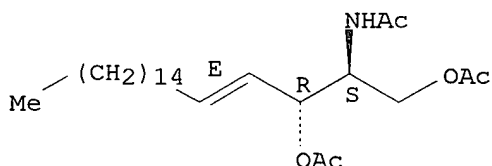
AB The stereochem. and synthetic utility of the addn. of 2-
 (trimethylsilyl)thiazole (I) to various N-protected .alpha.-amino
 aldehydes is described. The reactions of I with N-Boc-L-serinal acetonide
 (BOC = tert-butoxycarbonyl) (II) and N-Boc-L-threoninal acetonide are
 essentially anti diastereoselective (ds = 85-90%) in agreement with the
 Felkin-Anh model for asym. induction, whereas the reactions with
 O-benzyl-NH-Boc-L-serinal and NH-Boc-L-phenylalaninal are syn
 diastereoselective (ds = 80%). The reversal of diastereoselectivity is
 interpreted on the basis of a proton-bridged cyclic Cram model for asym.
 induction. The anti adduct III (R = 2-thiazolyl) derived from II was
 subjected to thiazole-to-formyl unmasking to give a one-carbon higher
 homolog II (R = CHO). This material serves as a precursor to ribo- and
 arabino-4-amino-4-deoxypentoses via a further one-carbon-chain elongation
 with I and to a C20 sphingosine via Wittig olefination. The above
 ribo-amino sugar was transformed via sequential Wittig olefination and
 redn. into a C18 phytosphingosine.

IT 25494-35-3P

Searched by Barb O'Bryen & Toby Port

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 RN 25494-35-3 CAPLUS
 CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-nonadecenyl]-,
 [R-[R*,S*-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
 Double bond geometry as shown.



L32 ANSWER 39 OF 72 CAPLUS COPYRIGHT 2000 ACS
 ACCESSION NUMBER: 1990:56573 CAPLUS
 DOCUMENT NUMBER: 112:56573
 TITLE: Preparation of sphingosine derivatives as antitumor agents
 INVENTOR(S): Sugimoto, Hirohiko; Sugawara, Tamio; Makino, Itsuo;
 Sato, Kozaburo; Narisada, Masayuki
 PATENT ASSIGNEE(S): Shionogi and Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 51 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 01093562	A2	19890412	JP 1987-252276	19871005
JP 2588729	B2	19970312		

OTHER SOURCE(S): MARPAT 112:56573

AB R1OCH2CHACH(OR2)CH:CH(CH2)nMe [I; R1 = H, acyl, glycosyl, phosphoric acid ester residue; R2 = H, acyl, glycosyl; A = (substituted) amino, N3; n = 10-14 integer], useful as antitumor agents and potentially useful for treatment of wounds and ulcers, are prepd. (2S,3R)-(Z)-HOCH2CH(NH2)CH(OH)CH:CH(CH2)12Me was acetylated with Ac2O to give (2S,3R)-(Z)-HOCH2CH(NHAc)CH(OH)CH:CH(CH2)12Me. In an in vivo study using MH 134 mouse tumor cells, 17 tested I at 2 mg i.p. showed 11->223% increase in life span of mice. About 40 I were prepd. with data.

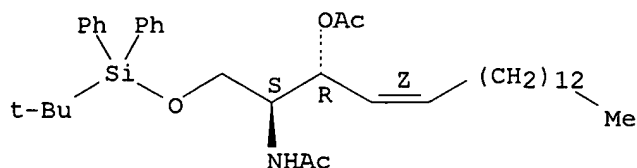
IT **123446-95-7**

RL: RCT (Reactant)
 (reaction of, in prepn. of antitumor sphingosine derivs.)

RN 123446-95-7 CAPLUS

CN Acetamide, N-[2-(acetyloxy)-1-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]methyl]-3-heptadecenyl]-, [R-[R*,S*-(Z)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
 Double bond geometry as shown.



L32 ANSWER 40 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1990:36288 CAPLUS

DOCUMENT NUMBER: 112:36288

TITLE: Synthesis of D-erythro-1-deoxydihydroceramide-1-sulfonic acid and phosphosphingoglycolipid found in marine organisms via a common precursor

AUTHOR(S): Ohashi, Kinji; Kosai, Shunji; Arizuka, Mitsuo; Watanabe, Takashi; Yamagiwa, Yoshiro; Kamikawa, Tadao; Kates, Morris

CORPORATE SOURCE: Fac. Sci. Technol., Kinki Univ., Higashi-Osaka, 577, Japan

SOURCE: Tetrahedron (1989), 45(9), 2557-70

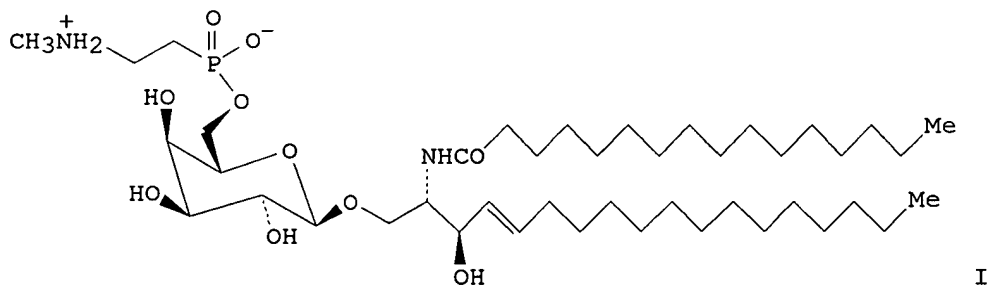
CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE: Journal

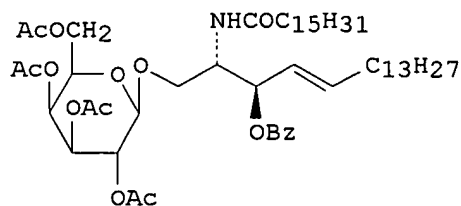
LANGUAGE: English

OTHER SOURCE(S): CASREACT 112:36288

GI



I



II

AB Galactopyranosylsphingosine deriv. I was prepd. from protected glycoside II in several steps. A sphingosine deriv. was converted to II.

IT 2482-37-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

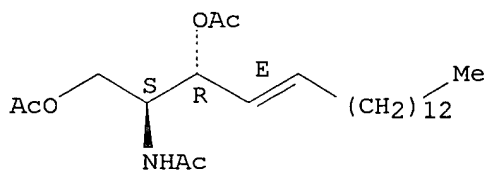
RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

Double bond geometry as shown.

Searched by Barb O'Bryen & Toby Port



L32 ANSWER 41 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1989:439825 CAPLUS

DOCUMENT NUMBER: 111:39825

TITLE: Unnatural ceramide-related compounds and their preparation as intermediates for sphingoglycolipids

INVENTOR(S): Fujita, Shuji; Yoshimura, Shoji; Ito, Masayoshi; Shitori, Yoshiyasu; Ogawa, Tomoya

PATENT ASSIGNEE(S): MECT Corp., Japan

SOURCE: Eur. Pat. Appl., 31 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

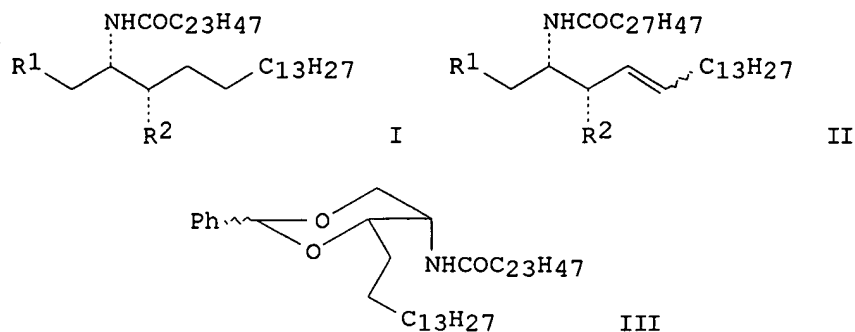
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 293006	A1	19881130	EP 1988-108537	19880527
EP 293006	B1	19910612		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
JP 63297351	A2	19881205	JP 1987-132696	19870528
CA 1314052	A1	19930302	CA 1988-567227	19880519
IL 86487	A1	19920818	IL 1988-86487	19880525
AU 8816664	A1	19881201	AU 1988-16664	19880526
AU 608851	B2	19910418		
US 4880572	A	19891114	US 1988-199107	19880526
HU 46655	A2	19881128	HU 1988-2715	19880527
HU 200995	B	19900928		
DK 8802923	A	19881129	DK 1988-2923	19880527
FI 8802507	A	19881129	FI 1988-2507	19880527
NO 8802342	A	19881129	NO 1988-2342	19880527
AT 64371	E	19910615	AT 1988-108537	19880527
HU 205894	B	19920728	HU 1990-3056	19880527
ES 2037763	T3	19930701	ES 1988-108537	19880527
CN 1031077	A	19890215	CN 1988-103176	19880528
CN 1013440	B	19910807		

PRIORITY APPLN. INFO.: JP 1987-132696 19870528
EP 1988-108537 19880527

OTHER SOURCE(S): MARPAT 111:39825

GI



AB Unnatural ceramide related compds. (I and II; R1, R2 = OH, AcO, EtOCH2CH2O), useful as intermediates for sphingoglycolipids, were prepd., e.g. by deacylation of a benzylideneoctadecanediol deriv. (III). Thus, azidolysis (37.6%) of (2R, 3S)-1,3-O-benzylidene-2-O-methanesulfonyl-4-octadecene-1,2,3-triol with NaN3 in DMF at 100-110.degree., hydrogenation (38.8%) of the resulting (2S, 3S, 4E)- and (2S, 3S, 4Z)-2-azido-1,3-O-benzylidene-4-octadecene-1,3-diol over 10% Pd-C, and acylation (36.8%) of the product amine with lignoceric acid in the presence of 2-chloro-1-methylpyridinium iodide and Bu3N in CH2Cl2 gave III. Refluxing III in CH2Cl2-MeOH (1:1) contg. Amberlyst-15 gave 72.4% I (R1 = R2 = OH).

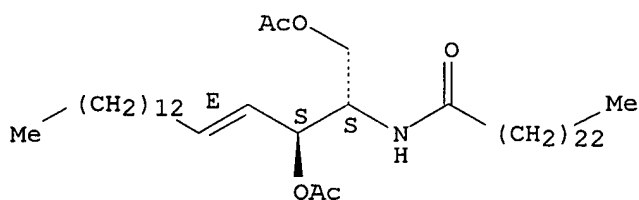
IT 121468-17-5P 121468-18-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as intermediate for glycosphingolipids)

RN 121468-17-5 CAPLUS

CN Tetracosanamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-,
[S-[R*,R*-(E)]]- (9CI) (CA INDEX NAME)

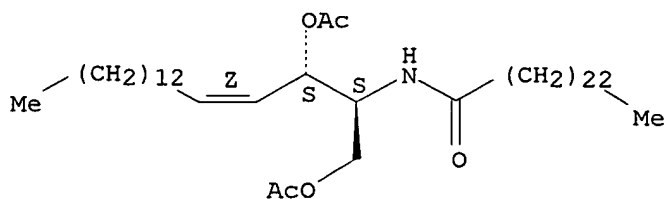
Absolute stereochemistry.
Double bond geometry as shown.



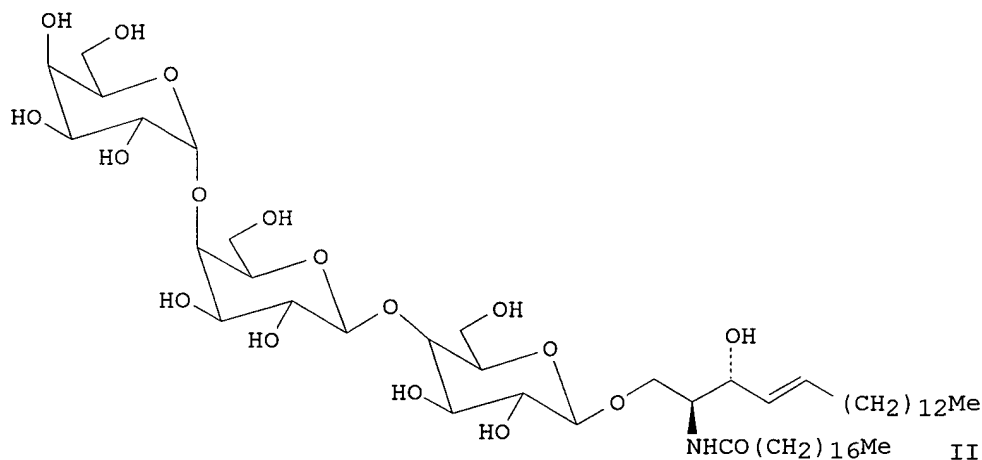
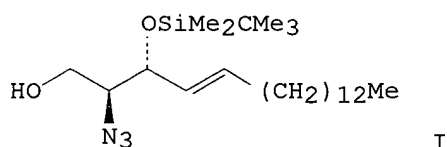
RN 121468-18-6 CAPLUS

CN Tetracosanamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-, [S-[R*,R*-(Z)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L32 ANSWER 42 OF 72 CAPLUS COPYRIGHT 2000 ACS
 ACCESSION NUMBER: 1989:8506 CAPLUS
 DOCUMENT NUMBER: 110:8506
 TITLE: A practical and enantioselective synthesis of
 glycosphingolipids and related compounds. Total
 synthesis of globotriaosylceramide (Gb3)
 AUTHOR(S): Nicolaou, K. C.; Caulfield, T.; Kataoka, H.; Kumazawa,
 T.
 CORPORATE SOURCE: Dep. Chem., Univ. Pennsylvania, Philadelphia, PA,
 19104, USA
 SOURCE: J. Am. Chem. Soc. (1988), 110(23), 7910-12
 CODEN: JACSAT; ISSN: 0002-7863
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 110:8506
 GI



AB Glycosphingolipids were prepd. enantioselectively via prepn. of
 enantiomerically pure sphingosine equiv. I and its coupling to suitable
 carbohydrate donors utilizing the two-stage activation glycosidation
 procedure. This efficient method is demonstrated by the construction of
 galactosylceramide, lactosylceramide and Gb3, (II).

IT **2482-37-3P**

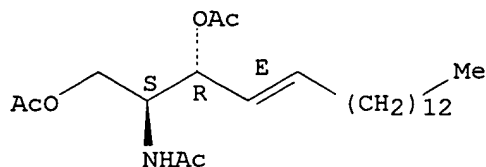
RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

RN 2482-37-3 CAPLUS

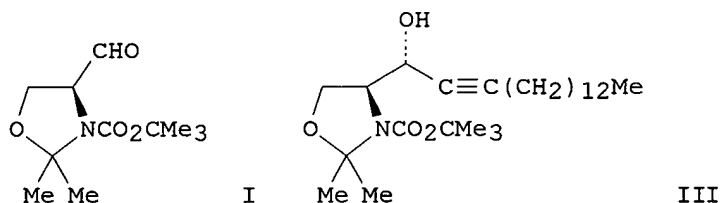
CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-
 heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

Double bond geometry as shown.



L32 ANSWER 43 OF 72 CAPLUS COPYRIGHT 2000 ACS
 ACCESSION NUMBER: 1988:630620 CAPLUS
 DOCUMENT NUMBER: 109:230620
 TITLE: Synthesis of D-erythro- and D-threo-sphingosine derivatives from L-serine
 AUTHOR(S): Herold, Peter
 CORPORATE SOURCE: Zent. Forschungslab., Ciba-Geigy A.-G., Basel, CH-4002, Switz.
 SOURCE: Helv. Chim. Acta (1988), 71(2), 354-62
 CODEN: HCACAV; ISSN: 0018-019X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 109:230620
 GI

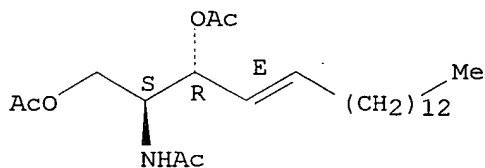


AB The protected serine aldehyde I was converted to the title cryst.
 N-protected sphingosines HOCH₂CH(NHR)CH(OH)CH:CH(CH₂)₁₂Me [II, R = Me₃CO₂C (Boc)] by a three-step reaction sequence. I was transformed with high diastereoselectivity (95%) either to the erythro- or threo-alkynols III. erythro-III is formed by the addn. of LiC.tplbond.C(CH₂)₁₂Me in THF/HMP at -78.degree., whereas the corresponding threo-III is produced in the presence of ZnBr₂ in Et₂O. Deprotection of the acetal moiety afforded the corresponding 1,3-diols. These diols were selectively reduced with Red-Al to the (E)-sphingosines II, or the Z-isomers by partial hydrogenation over Lindlar's catalyst. Cleavage of the N-Boc group and further transformation to ceramides were readily achieved as demonstrated by the conversion of (E)-erythro-II (R = Boc) to N-octadecanoyl-D-erythro-sphingosine II [R = CO(CH₂)₁₆Me].

IT **2482-37-3P 78779-96-1P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 RN 2482-37-3 CAPLUS
 CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).
 Double bond geometry as shown.

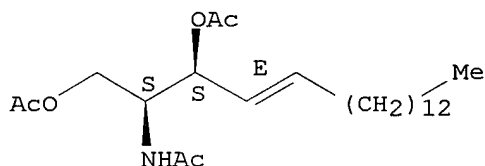
Searched by Barb O'Bryen & Toby Port



RN 78779-96-1 CAPLUS

CN Acetamide, N-[(1S,2S,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



L32 ANSWER 44 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1988:590104 CAPLUS

DOCUMENT NUMBER: 109:190104

TITLE: Synthesis of D-erythro-1-deoxydihydroceramide-1-sulfonic acid

AUTHOR(S): Ohashi, Kinji; Yamagiwa, Yoshiro; Kamikawa, Tadao; Kates, Morris

CORPORATE SOURCE: Fac. Sci. Technol., Kinki Univ., Higashi-Osaka, Japan

SOURCE: Tetrahedron Lett. (1988), 29(10), 1185-8

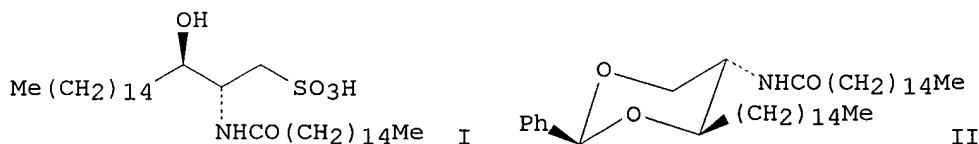
CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 109:190104

GI



AB New D-erythro-1-deoxydihydroceramide-1-sulfonic acid (I), isolated from alkali-stable lipids in a non-photosynthetic marine diatom, *Nitzschia alba*, was synthesized from galactose as a chiral precursor using the reaction of acetal II with NBS-BaCO₃ in CCl₄ as the key step in the reaction sequence.

IT 2482-37-3P

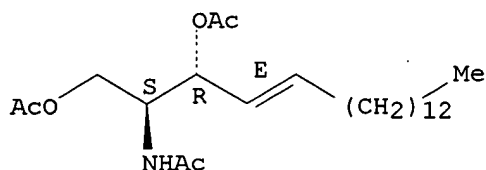
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Searched by Barb O'Bryen & Toby Port

Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.



L32 ANSWER 45 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1988:549902 CAPLUS

DOCUMENT NUMBER: 109:149902

TITLE: Synthesis of a phosphosphingoglycolipid found in the marine snail Turbo cornutus

AUTHOR(S): Ohashi, Kinji; Kosai, Shunji; Arizuka, Mitsuo;

Watanabe, Takashi; Fukunaga, Mikio; Monden, Koji;

Uchikoda, Takao; Yamagiwa, Yoshiro; Kamikawa, Tadao

CORPORATE SOURCE: Fac. Sci. Technol., Kinki Univ., Higashi-Osaka, Japan

SOURCE: Tetrahedron Lett. (1988), 29(10), 1189-92

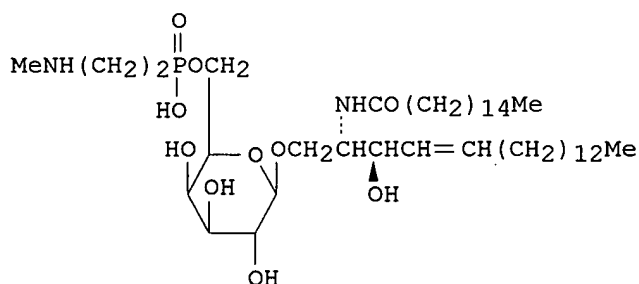
CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal

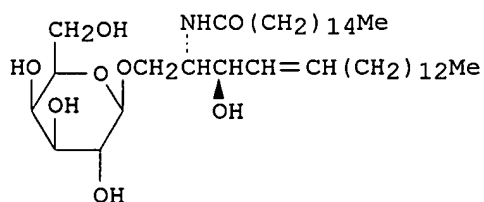
LANGUAGE: English

OTHER SOURCE(S): CASREACT 109:149902

GI



I



II

AB The phosphosphingoglycolipid I is synthesized from galactose as a chiral precursor via condensation of cerebroside II with (HO)₂P(O)CH₂CH₂NMeCO₂CH₂CCl₃ using EDCI as the key step.

IT 116448-00-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and benzylation of)

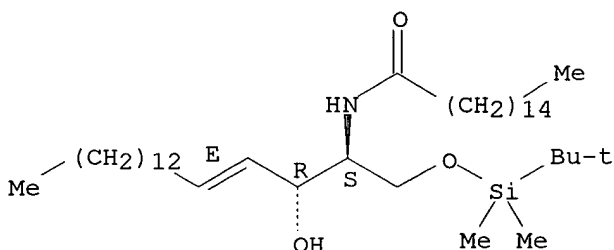
RN 116448-00-1 CAPLUS

CN Hexadecanamide, N-[1-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-2-hydroxy-3-heptadecenyl]-, [R-[R*,S*-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Searched by Barb O'Bryen & Toby Port

Double bond geometry as shown.



L32 ANSWER 46 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1988:549173 CAPLUS

DOCUMENT NUMBER: 109:149173

TITLE: Asymmetric synthesis of threo- and erythro-sphingosines by asymmetric aldol reaction of .alpha.-isocyanoacetate catalyzed by a chiral ferrocenylphosphine gold(I) complex

AUTHOR(S): Ito, Yoshihiko; Sawamura, Masaya; Hayashi, Tamio

CORPORATE SOURCE: Dep. Synth. Chem., Kyoto Univ., Kyoto, 606, Japan

SOURCE: Tetrahedron Lett. (1988), 29(2), 239-40

CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 109:149173

AB Asym. aldol reaction of CNCH₂CO₂Me with (E)-2-hexadecenal in the presence of 1 mol% of a chiral (aminoalkyl)ferrocenylphosphine-gold(I) complex gave optically active trans-4-(methoxycarbonyl)-5-[(E)-1-pentadecenyl]-2-oxazoline which was readily converted into D-threo- and erythro-sphingosines.

IT 116612-39-6P

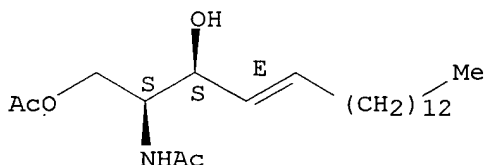
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and Mitsunobu reaction of)

RN 116612-39-6 CAPLUS

CN Acetamide, N-[1-[(acetyloxy)methyl]-2-hydroxy-3-heptadecenyl]-, [S-[R*,R*-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



IT 2482-37-3P 78779-96-1P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

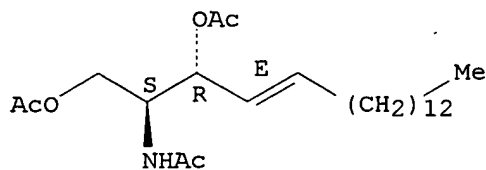
RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

Double bond geometry as shown.

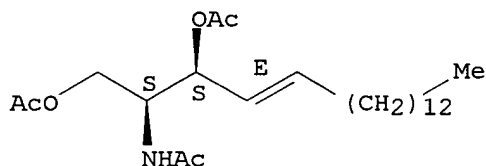
Searched by Barb O'Bryen & Toby Port



RN 78779-96-1 CAPLUS

CN Acetamide, N-[(1S,2S,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



L32 ANSWER 47 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1988:510149 CAPLUS

DOCUMENT NUMBER: 109:110149

TITLE: A stereodivergent synthesis of D-erythro-sphingosine and D-threo-sphingosine from L-serine

AUTHOR(S): Garner, Philip; Park, Jung Min; Malecki, Elise

CORPORATE SOURCE: Dep. Chem., Case West. Reserve Univ., Cleveland, OH, 44106-2699, USA

SOURCE: J. Org. Chem. (1988), 53(18), 4395-8

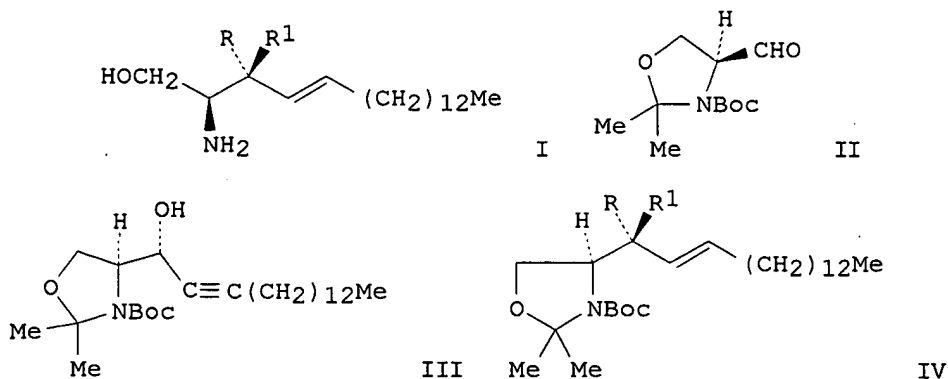
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 109:110149

GI



AB The stereocontrolled synthesis of both D-erythro-sphingosine I (R = OH, R1 = H) and D-threo-sphingosine I (R = H, R1 = OH) from L-serine-derived
Searched by Barb O'Bryen & Toby Port

oxazolidine aldehyde II (Boc = CO₂Me₃) is described. Addn. of LiC.tplbond.C(CH₂)₁₂Me to II proceeded with very good diastereoselectivity to give the erythro propargylic alc. III as expected for a non-chelated transition state. Redn. of III with lithium in ethylamine at -78.degree. resulted in clean redn. of the triple bond producing the protected sphingosine deriv. IV (R= OH, R₁= H; V). Hydrolysis of this material with 1N HCl followed by extractive isolation and trituration led to the formation of I (R= OH, R₁=H) in 65% overall yield from II. Prolonged exposure of V to lithium in ethylamine resulted in a novel fragmentation of the N-Boc oxazolidine moiety to give I directly in 68% overall yield after similar workup and recrystn. However, the addn. of (Me₂CHCH₂)₂ AlCH:CH(CH₂)₁₂Me to II resulted in the moderately selective formation of threo allylic alc. IV (R= H, R₁= OH) resulting from an .alpha.-chelation controlled transition state. This material was hydrolyzed with 1 N HCl to give a (2:1) mixt. of I (R, R₁ = H, OH) in 60% overall yield.

IT 2482-37-3P 78779-96-1P

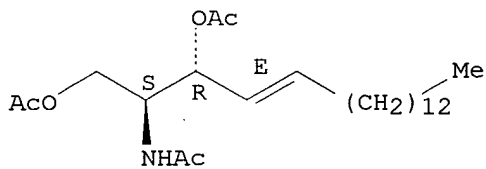
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

Double bond geometry as shown.

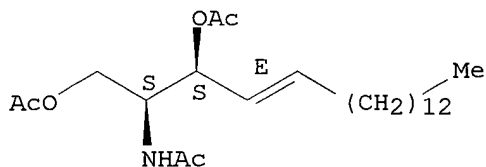


RN 78779-96-1 CAPLUS

CN Acetamide, N-[(1S,2S,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

Double bond geometry as shown.



L32 ANSWER 48 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1988:493486 CAPLUS

DOCUMENT NUMBER: 109:93486

TITLE: Stereoselective mono- and bis-homologation of
L-serinal via 2-(trimethylsilyl)thiazole addition.
Thiazole route to amino L-sugars and
D-erythro-sphingosines

AUTHOR(S): Dondoni, Alessandro; Fantin, Giancarlo; Fogagnolo,
Marco; Medici, Alessandro

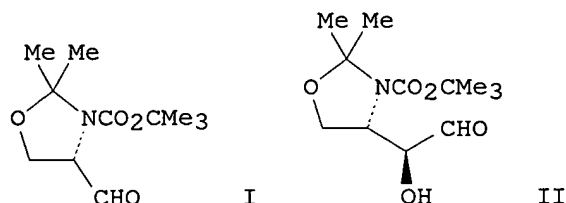
CORPORATE SOURCE: Dip. Chim., Univ. Ferrara, Ferrara, Italy

SOURCE: J. Chem. Soc., Chem. Commun. (1988), (1), 10-12
CODEN: JCCCAT; ISSN: 0022-4936

DOCUMENT TYPE: Journal

Searched by Barb O'Bryen & Toby Port

LANGUAGE: English
 OTHER SOURCE(S): CASREACT 109:93486
 GI



AB Anti-addn. [92% diastereoselectivity] of 2-trimethylsilylthiazole to O,N-protected L-serinal (I) and deblocking the formyl group in the resulting adduct, leads to the (2S,3S)-2,4-dihydroxy-3-aminobutanal deriv. (II), which serves as a precursor both to masked 4-amino-4-deoxy-L-ribose/L-arabinose and D-erythro-C20-sphingosine.

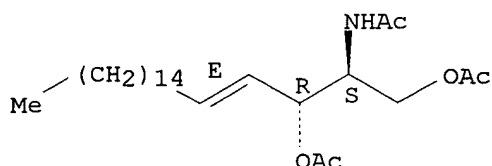
IT **25494-35-3P**

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

RN 25494-35-3 CAPLUS

CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-nonadecenyl]-,
 [R-[R*,S*-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
 Double bond geometry as shown.



L32 ANSWER 49 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1987:420303 CAPLUS

DOCUMENT NUMBER: 107:20303

TITLE: Fumarase-catalyzed synthesis of L-threo-chloromalic acid and its conversion to 2-deoxy-D-ribose and D-erythro-sphingosine

AUTHOR(S): Findeis, Mark A.; Whitesides, George M.

CORPORATE SOURCE: Dep. Chem., Harvard Univ., Cambridge, MA, 02138, USA

SOURCE: J. Org. Chem. (1987), 52(13), 2838-48

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The use is described of pig heart fumarase (EC 4.2.1.2) as a catalyst in the multigram synthesis of L-threo-chloromalic acid (I) (.gtoreq.99.5% enantiomeric excess) on 50-g scale. L-threo-Fluoromalic acid has been synthesized in a coupled enzymic system from difluorofumaric acid. I serves as starting material for synthesis of 2-deoxy-D-ribose and D-erythro-sphingosine.

IT **2482-37-3P**

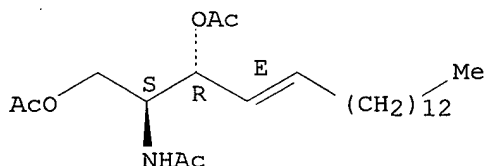
RL: PREP (Preparation)
 (prepn. of)

RN 2482-37-3 CAPLUS

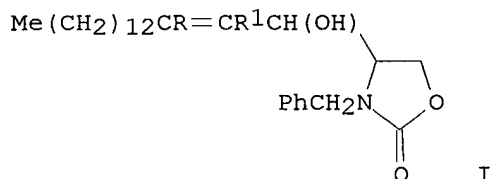
CN Acetamide, N-[(1S,2R,3E)-2-(acetvloxv)-1-[(acetvloxv)methyl]-3-
 Searched by Barb O'Bryen & Toby Port

heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.



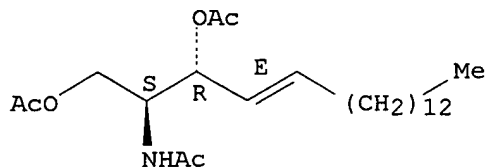
L32 ANSWER 50 OF 72 CAPLUS COPYRIGHT 2000 ACS
 ACCESSION NUMBER: 1986:626155 CAPLUS
 DOCUMENT NUMBER: 105:226155
 TITLE: Enantioselective synthesis of D-erythro-sphingosine
 and of ceramide
 AUTHOR(S): Julina, Radomir; Herzig, Thomas; Bernet, Bruno;
 Vasella, Andrea
 CORPORATE SOURCE: Org.-Chem. Inst., Univ. Zurich, Zurich, CH-8057,
 Switz.
 SOURCE: Helv. Chim. Acta (1986), 69(2), 368-73
 CODEN: HCACAV; ISSN: 0018-019X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 105:226155
 GI



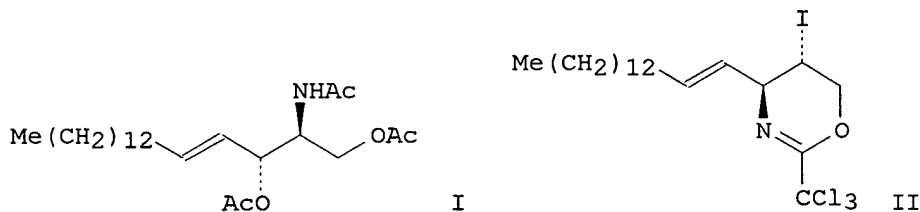
AB (E)-HC.tplbond.CCH:CHCH₂OH was transformed into D-erythro-sphingosine in 7 steps and 46% overall yield and into ceramide in 8 steps and 41% overall yield. The key steps were the mono-epoxidn. of Me(CH₂)₁₂C.tplbond.CCH:CHCH₂OH (by Ti(OCMe₃)₄, di-Et (-)-D-tartrate, and Me₃COOH) to the (R,R)-epoxide (86%, .gtoreq.98% enantiomeric excess), the regioselective intramol. opening of the oxirane via the benzylurethane, and the reductive transformation of the acetylene I (RR₁ = bond) into the oxazolidinone I (R = R₁ = H).

IT **2482-37-3P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 RN 2482-37-3 CAPLUS
 CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.



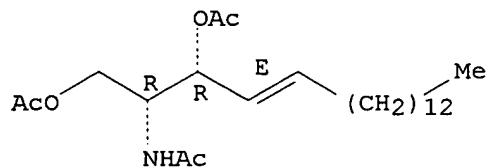
L32 ANSWER 51 OF 72 CAPLUS COPYRIGHT 2000 ACS
 ACCESSION NUMBER: 1986:590762 CAPLUS
 DOCUMENT NUMBER: 105:190762
 TITLE: A novel, efficient synthesis of (.+-.)-erythro-sphingosine
 AUTHOR(S): Cardillo, Giuliana; Orena, Mario; Sandri, Sergio; Tomasini, Claudia
 CORPORATE SOURCE: Cent. Stud. Fis. Macromol., Ist. Chim. "G. Ciamician", Bologna, 40126, Italy
 SOURCE: Tetrahedron (1986), 42(3), 917-22
 CODEN: TETRAB; ISSN: 0040-4020
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 105:190762
 GI



AB In a stereoselective synthesis of (.+-.)-erythro-sphingosine triacetate (I) the key reaction that detes. the right stereochem. is the iodocyclization of (2E,4E)-Me(CH₂)₁₂(CH:CH)2CH₂OC(:NH)CCl₃ to the 4,5-dihydro-1,3-oxazine II. Cleavage of II with HCl and treatment with Amberlyst A 26 in the AcO- form, followed by full acetylation, affords I in good yield.

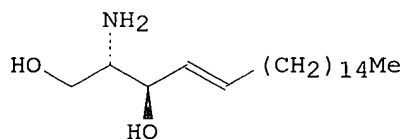
IT **86161-75-3P**
 RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)
 RN 86161-75-3 CAPLUS
 CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-, [R*,R*-(E)]- (9CI) (CA INDEX NAME)

Relative stereochemistry.
 Double bond geometry as shown.



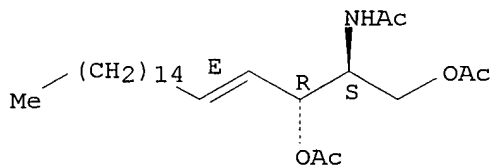
Searched by Barb O'Bryen & Toby Port

L32 ANSWER 52 OF 72 CAPLUS COPYRIGHT 2000 ACS
 ACCESSION NUMBER: 1986:460459 CAPLUS
 DOCUMENT NUMBER: 105:60459
 TITLE: Synthesis of sphingosines. Part 2. Synthesis of D-erythro-sphingosines
 AUTHOR(S): Schmidt, Richard R.; Zimmermann, Peter
 CORPORATE SOURCE: Fak. Chem., Univ. Konstanz, Konstanz, D-7750, Fed. Rep. Ger.
 SOURCE: Tetrahedron Lett. (1986), 27(4), 481-4
 CODEN: TELEAY; ISSN: 0040-4039
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 105:60459
 GI



AB 2,4-Di-O-protected D-threose, readily available from D-galactose, is a versatile intermediate for D-erythro-sphingosine, e.g., I, syntheses via trans-selective Wittig reaction, aside introduction at the unprotected hydroxylic group, and subsequent aside redn.
 IT **25494-35-3P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 RN 25494-35-3 CAPLUS
 CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-nonadecenyl]-, [R-[R*,S*-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
 Double bond geometry as shown.



L32 ANSWER 53 OF 72 CAPLUS COPYRIGHT 2000 ACS
 ACCESSION NUMBER: 1986:221553 CAPLUS
 DOCUMENT NUMBER: 104:221553
 TITLE: Complete structural analysis of globoseries glycolipids by two-dimensional nuclear magnetic resonance
 AUTHOR(S): Gasa, Shinsei; Nakamura, Mitsuru; Makita, Akira; Ikura, Mitsuhiko; Hikichi, Kunio
 CORPORATE SOURCE: Sch. Med., Hokkaido Univ., Sapporo, 060, Japan
 SOURCE: Eur. J. Biochem. (1986), 155(3), 603-11
 CODEN: EJBCAI; ISSN: 0014-2956
 DOCUMENT TYPE: Journal
 Searched by Barb O'Bryen & Toby Port

LANGUAGE: English

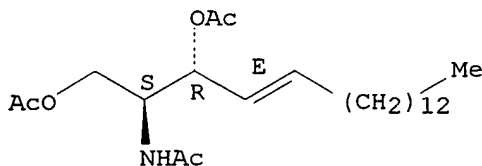
AB Combined 2-dimensional proton NMR allowed the detn. of complete oligosaccharide structures of glycolipids belonging to the globo series, without any other anal. methods. Although a chem. modification by peracetylation was required for the above purpose, the derivatization permitted facile assignment of the pyranose ring proton resonances of the oligosaccharide moiety. Two-dimensional chem.-shift-correlated spectroscopy of the acetylated glycolipid enabled elucidation the glycosidic positions from the chem. shifts of the protons at the substituted sites. The monosaccharide species were also identified from the characteristic splitting patterns of the methine protons on individual pyranose rings. The sequence of the monosaccharides was inferred from the interresidue connectivity across glycosidic linkages shown by 2-dimensional nuclear Overhauser effect spectroscopy, which also gave intraresidue interaction on the pyranose rings. The linkage sites of long oligosaccharide chains having more than 5 monosaccharides, such as globopentaosylceramide, were analyzed by 2-dimensional J-relayed coherence transfer, which yielded 1,3 interactions along with 1,2 interactions.

IT 2482-37-3

RL: PRP (Properties)
(NMR spectrum of)

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.

L32 ANSWER 54 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1985:23726 CAPLUS

DOCUMENT NUMBER: 102:23726

TITLE: Diastereoselective synthesis of unsaturated vicinal amino alcohols via Diels-Alder reactions of N-sulfinyl dienophiles

AUTHOR(S): Garigipati, Ravi S.; Freyer, Alan J.; Whittle, Robert R.; Weinreb, Steven M.

CORPORATE SOURCE: Dep. Chem., Pennsylvania State Univ., University Park, PA, 16802, USA

SOURCE: J. Am. Chem. Soc. (1984), 106(25), 7861-7

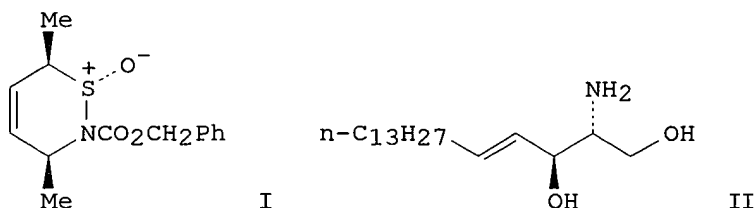
CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 102:23726

GI



AB .alpha.-Hydroxy-.beta.,.gamma.-unsatd. amine derivs. were synthesized from 3,6-dihydrothiazine 1-oxides, which were obtained stereoselectively by Diels-Alder [4 + 2] cycloaddn. of N-sulfinyl dienophiles and 1,3-dienes of known geometry. Fission of the S-N bond of the adduct with a Grignard reagent led to allylic sulfoxides which were converted stereoselectively to allyl alcs. via an allylic sulfoxide/sulfenate ester [2,3]-sigmatropic rearrangement. (E,E)- And (E,Z)-2,4-hexadiene were stereoselectively transformed to threo- and erythro-MeCH:CHCH(OH)CHMeNHCO2CH2Ph. Intermediates in these transformations were investigated by 1H NMR expts. The configuration and conformation of Diels-Alder adduct I were detd. by x-ray crystallog. and 1H NMR lanthanide induced shift expts. A variation of this strategy incorporating intramol. N-sulfinyl Diels-Alder reactions was used in the total synthesis of the sphingolipid bases erythro- (II) and threo-sphingosine.

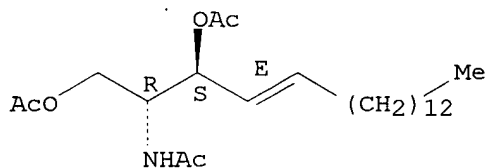
IT **67113-24-0P 86161-75-3P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 67113-24-0 CAPLUS

CN Acetamide, N-[(1R,2S,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-, rel- (9CI) (CA INDEX NAME)

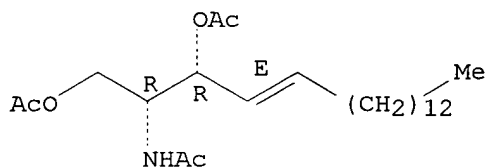
Relative stereochemistry.
Double bond geometry as shown.



RN 86161-75-3 CAPLUS

CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-, [R*,R*-(E)]- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



L32 ANSWER 55 OF 72 CAPLUS COPYRIGHT 2000 ACS

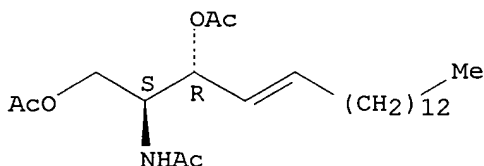
ACCESSION NUMBER: 1984:120758 CAPLUS

DOCUMENT NUMBER: 100:120758

Searched by Barb O'Bryen & Toby Port

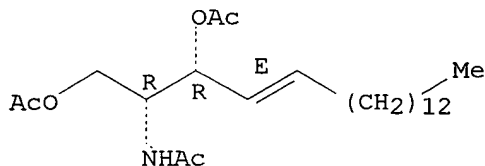
TITLE: Enantioselective synthesis of D-erythro-sphingosine
 AUTHOR(S): Bernet, Bruno; Vasella, Andrea
 CORPORATE SOURCE: Org. Chem. Inst., Univ. Zurich, Zurich, CH-8057, Switz.
 SOURCE: Tetrahedron Lett. (1983), 24(49), 5491-4
 CODEN: TELEAY; ISSN: 0040-4039
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB D-erythro-Sphingosine [Me(CH₂)₁₂CH:CH(OH)CH(NH₂)CH₂OH, I] and the L-erythro isomer Me(CH₂)₁₂CH:CH(NH₂)CH(OH)CH₂OH were synthesized in a highly enantio- and regioselective manner by a modified Sharpless asym. epoxidn. The overall yield of I from CH.tplbond.C(CH₂)₁₂Me in 6 steps was 33%.
 IT **89164-22-7P**
 RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)
 RN 89164-22-7 CAPLUS
 CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
 Double bond geometry unknown.



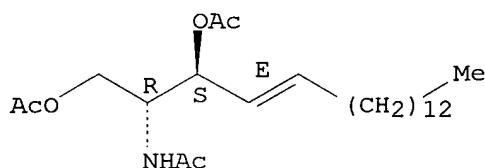
L32 ANSWER 56 OF 72 CAPLUS COPYRIGHT 2000 ACS
 ACCESSION NUMBER: 1983:438288 CAPLUS
 DOCUMENT NUMBER: 99:38288
 TITLE: Stereospecific synthesis of acyclic unsaturated amino alcohols. A new approach to threo and erythro sphingosine
 AUTHOR(S): Garigipati, Ravi S.; Weinreb, Steven M.
 CORPORATE SOURCE: Dep. Chem., Pennsylvania State Univ., University Park, PA, 16802, USA
 SOURCE: J. Am. Chem. Soc. (1983), 105(13), 4499-501
 CODEN: JACSAT; ISSN: 0002-7863
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB A new stereospecific synthesis of .alpha.-hydroxy-.beta.,.gamma.-unsatd. acyclic amines is based upon an initial stereospecific Diels-Alder cycloaddn. of PhCH₂O₂CN:SO with a 1,3-diene of known geometry, followed by conversion of the product to an allylic sulfoxide with PhMgBr. A stereospecific [2,3]-sigmatropic rearrangement of the allylic sulfoxide affords the desired unsatd. vicinal amino alc. This route has been applied to (E,E) and (E,Z)-MeCH:CHCH:CHMe to afford MeCH:CHCH(OH)CHMeNHCO₂CH₂Ph with total stereocontrol. The method has also been used in syntheses of threo- and erythro-sphingosine. A key strategy in these routes involves the first examples of intramol. N-sulfinyl-imine Diels-Alder processes.
 IT **86161-75-3P**
 RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)
 RN 86161-75-3 CAPLUS
 CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-, [R*,R*-(E)]- (9CI) (CA INDEX NAME)
 Searched by Barb O'Bryen & Toby Port

Relative stereochemistry.
Double bond geometry as shown.



L32 ANSWER 57 OF 72 CAPLUS COPYRIGHT 2000 ACS
 ACCESSION NUMBER: 1982:217554 CAPLUS
 DOCUMENT NUMBER: 96:217554
 TITLE: Diastereoselective synthesis of D,L-sphingosine
 AUTHOR(S): Schmidt, Richard R.; Klaeger, Rudolf
 CORPORATE SOURCE: Fak. Chem., Univ. Konstanz, Konstanz, D-7750, Fed. Rep. Ger.
 SOURCE: Angew. Chem. (1982), 94(3), 215-16
 CODEN: ANCEAD; ISSN: 0044-8249
 DOCUMENT TYPE: Journal
 LANGUAGE: German
 AB DL-Sphingosine was prepd. by reaction of Me(CH₂)₁₂CH:CHCHO with (Me₃Si)NCH₂CO₂SiMe₃ and LiAlH₄ redn. of Me(CH₂)₁₂CH:CHCH(OH)CH(NH₂)CO₂H.
 IT 67113-24-0P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and deacetylation of)
 RN 67113-24-0 CAPLUS
 CN Acetamide, N-[(1R,2S,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



L32 ANSWER 58 OF 72 CAPLUS COPYRIGHT 2000 ACS
 ACCESSION NUMBER: 1981:569690 CAPLUS
 DOCUMENT NUMBER: 95:169690
 TITLE: Useful syntheses of erythro- and threo-N-oleoyl-D-sphingosines (ceramides) and galactosylceramides (cerebrosides) from L-serine
 AUTHOR(S): Tkaczuk, Peter; Thornton, Edward R.
 CORPORATE SOURCE: Dep. Chem., Univ. Pennsylvania, Philadelphia, PA, 19104, USA
 SOURCE: J. Org. Chem. (1981), 46(22), 4393-8
 CODEN: JOCEAH; ISSN: 0022-3263
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The 4-(carbomethoxy)-2-phenyl-.DELTA.2-oxazoline formed from L-serine is the basis for a useful synthesis of ceramides and cerebrosides on the 100 mg scale with .apprx.100% optical purity. The natural erythro configuration and its threo epimer, formed in equal amts., are readily
 Searched by Barb O'Bryen & Toby Port

sepd. chromatog. so that both epimers are available for comparisons of the properties of erythro and threo configurations. The threo epimer and other analogs of the natural cerebroside with different chain lengths and stereochem. should be readily available by this method.

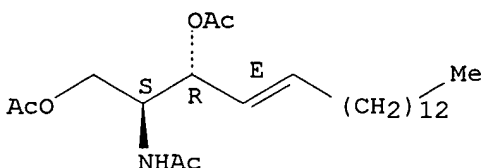
IT 2482-37-3P 78779-96-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

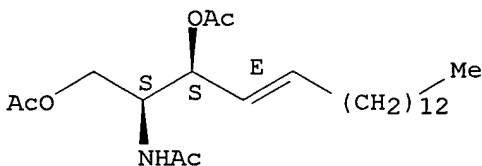
Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.



RN 78779-96-1 CAPLUS

CN Acetamide, N-[(1S,2S,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



L32 ANSWER 59 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1978:442300 CAPLUS

DOCUMENT NUMBER: 89:42300

TITLE: Total synthesis of stereospecific sphingosine and ceramide

AUTHOR(S): Shoyama, Yukihiro; Okabe, Hikaru; Kishimoto, Yasuo; Costello, Catherine

CORPORATE SOURCE: John F. Kennedy Inst., Johns Hopkins Sch. Med., Baltimore, Md., USA

SOURCE: J. Lipid Res. (1978), 19(2), 250-9

CODEN: JLPRAW; ISSN: 0022-2275

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Et DL-erythro-2-acetamino-3-hydroxy-4-trans-octadecenoate was esterified with L(+)-acetylmandeloyl chloride and the two diastereomers obtained were sepd. from each other by thin-layer or column chromatog. One of the isomers was subjected to ethanolysis to obtain Et D-erythro-2-amino-3-hydroxy-4-trans-octadecenoate which was then reduced with LiAlH₄ or NaBH₄ to yield D-erythro-sphingosine.

IT 2482-37-3P 67113-24-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

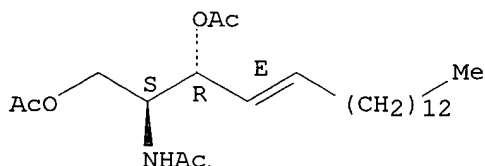
RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Searched by Barb O'Bryen & Toby Port

heptadecenyl]- (9CI) (CA INDEX NAME)

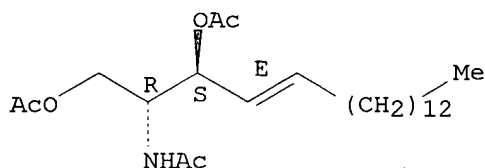
Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.



RN 67113-24-0 CAPLUS

CN Acetamide, N-[(1R,2S,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



L32 ANSWER 60 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1977:38979 CAPLUS

DOCUMENT NUMBER: 86:38979

TITLE: Molecular arrangements in sphingolipids. Conformation and hydrogen bonding of ceramide and their implication on membrane stability and permeability

AUTHOR(S): Pascher, Irmin

CORPORATE SOURCE: Fac. Med., Univ. Goteborg, Goteborg, Swed.

SOURCE: Biochim. Biophys. Acta (1976), 455(2), 433-51

CODEN: BBACAQ

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The preferred conformation of the ceramide part of sphingolipids was deduced from single crystal structures of a series of sphingolipid constituents: N-tetracosanoylphytosphingosine, glycosylphytosphingosine-HCl, sphingosine-HCl, triacetyl sphingosine, DL-2-hydroxytetradecanoic acid, and N-stearoylethanolamine. The amide group of the ceramide, which serves as a link between the hydrocarbon chains, has a basic significance for the conformation of the entire mol. This rigid group, which comprises 6 atoms in a planar conformation, adopts a perpendicular orientation towards the axes of the 2 hydrocarbon chains. The carbonyl O thereby turns into an eclipsed position with the H atom at C-2 of the sphingosine. A parallel chain stacking is achieved by a sharp perpendicular bend of the fatty acid. This bend is produced by a sequence of 2 -60.degree. rotations about the C-C bonds at both sides of the .alpha.-C atom. The orientation of the H bond donors and acceptors of the amide group and the hydroxyl groups allow lateral interaction with other lipid mols. The proposed models are supported by IR spectra, thin-layer chromatog. behavior, and monolayer studies of synthetic model ceramides. The functional role of the H bonding groups in the ceramide part of sphingolipids is emphasized and their significance for the formation of lateral H bonds within the membrane layer and thereof arising effects on membrane stability and permeability are discussed.

Searched by Barb O'Bryen & Toby Port

IT 25494-35-3

RL: PRP (Properties)

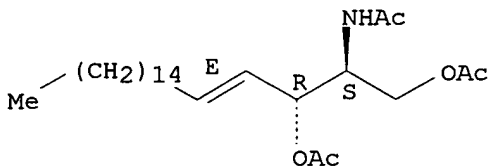
(crystal structure of, ceramide conformation in relation to)

RN 25494-35-3 CAPLUS

CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-nonadecenyl]-, [R-[R*,S*-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



L32 ANSWER 61 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1976:150300 CAPLUS

DOCUMENT NUMBER: 84:150300

TITLE: Synthesis of sphingomyelins via their dimethylamino precursors

AUTHOR(S): Zvonkova, E. N.; Mitsner, B. I.; Bushnev, A. S.; Orlova, E. G.; Gabor, Kruppa; Markina, N. N.; Talagaeva, S. V.; Evstigneeva, R. P.

CORPORATE SOURCE: M. V. Lomonosov Inst. Fine Chem. Technol., Moscow, USSR

SOURCE: Bioorg. Khim. (1975), 1(12), 1746-54
CODEN: BIKHD7

DOCUMENT TYPE: Journal

LANGUAGE: Russian

AB Sphingomyelins, based on trimethylammonio derivs. of sphingenine, rac-sphinganine, and threo-rac-sphinganine were prepd. 3-Benzoylceramide phosphoryldimethylaminoethyl derivs. were prepd. from 3-benzoylceramides via 2-chloroethylphosphoryl-3-benzoylceramides or 3-benzoylceramide phosphates. The 3-benzoylceramide prepn. was modified, and 3-benzoyl-rac-sphingenine sulfate was resolved with d-(+)-tartaric acid.

IT 2482-37-3P

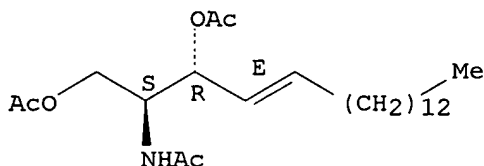
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

Double bond geometry as shown.



L32 ANSWER 62 OF 72 CAPLUS COPYRIGHT 2000 ACS

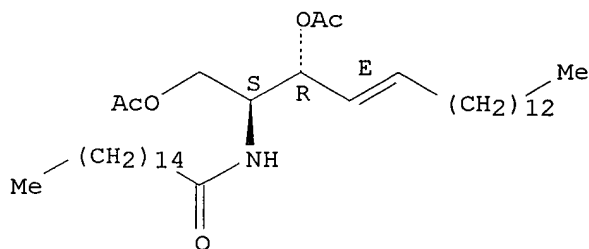
ACCESSION NUMBER: 1975:116603 CAPLUS

DOCUMENT NUMBER: 82:116603

TITLE: Monolayer studies on derivatives of sphinganine and
Searched by Barb O'Bryen & Toby Port

4t-sphingenine
 AUTHOR(S): Stoffel, W.; Pruss, H. D.; Sticht, G.
 CORPORATE SOURCE: Inst. Physiol. Chem., Univ. Koeln, Cologne, Ger.
 SOURCE: Chem. Phys. Lipids (1974), 13(4), 466-80
 CODEN: CPLIA4
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The pressure-area isotherms at 4-47.degree. of the following derivs. of sphinganine and 4t-sphingenine were detd.; N-palmitoyl-D,L-sphingenine (I), N-palmitoyldiacetyl-D,L-sphingenine (II), N-acetylsphingenine (III), N-acetyl-D,L-erythro-sphinganine (IV), N-acetyl-D,L-threo-sphinganine (V), triacetyl-D,L-erythro-sphinganine (VI), N-acetyl-3-dehydrosphingenine (VII), N-acetyl-3-dehydro-D,L-sphinganine (VIII) and diacetyl-3-dehydro-D,L-sphinganine (IX). The phases of the monolayer films are discussed. III, V, VI, VIII, and IX form trilayers when their monolayers are compressed beyond the collapse point. The folding to a trilayer is only possible from the liq. expanded state of the monolayer. The formation of trilayer films occur only when the area of the hydrophilic group exceeds that of the alkane chain of the long chain base.
 IT **54824-82-7**
 RL: PRP (Properties)
 (monolayers of)
 RN 54824-82-7 CAPLUS
 CN Hexadecanamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-, [R*,S*-(E)]- (9CI) (CA INDEX NAME)

Relative stereochemistry.
 Double bond geometry as shown.



L32 ANSWER 63 OF 72 CAPLUS COPYRIGHT 2000 ACS
 ACCESSION NUMBER: 1973:432244 CAPLUS
 DOCUMENT NUMBER: 79:32244
 TITLE: Structural studies on glycolipids. 1. 220 MHz PMR spectra of acetylated galactocerebrosides
 AUTHOR(S): Martin-Lomas, M.; Chapman, D.
 CORPORATE SOURCE: Biophys. Div., Unilever Res. Lab., Welwyn/Herts., Engl.
 SOURCE: Chem. Phys. Lipids (1973), 10(2), 152-64
 CODEN: CPLIA4
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The PMR spectra of fully acetylated 2-amino-trans-2S,3R-4-octadecene-1,3-diol (sphingosine), the dihydro deriv., 1-O-.beta.-D-galactopyranosyl-2-tetracosanoylamido-trans-2S,3R-4-octadecene-1,3-diol (cerasine), and 1-O-.beta.-D-galactopyranosyl-2-hydroxy-2-tetracosanoylamido-trans-2S,3R-4-octadecene-1,3-diol (phrenosine) were detd. in CDCl3, CD3COCD3 and benzene-d6 at 220 MHz. The relative chem. shifts of the protons in the three solvents permitted configurational and conformational detns.
 IT **2482-37-3**
 RL: RCT (Reactant)

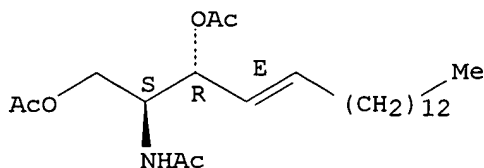
Searched by Barb O'Bryen & Toby Port

(PMR of, configuration in relation to)

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.



L32 ANSWER 64 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1973:68524 CAPLUS

DOCUMENT NUMBER: 78:68524

TITLE: Carbon-13-nuclear magnetic resonance spectroscopic studies on saturated, mono-, di-, and polyunsaturated fatty acids, phospho- and sphingolipids

AUTHOR(S): Stoffel, Wilhelm; Zierenberg, Ottfried; Tunggal, Budi D.

CORPORATE SOURCE: Inst. Physiol. Chem., Univ. Koeln, Cologne, Ger.

SOURCE: Hoppe-Seyler's Z. Physiol. Chem. (1972), 353(12), 1962-9

CODEN: HSZPAZ

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Complete and unequivocal ¹³C magnetic resonance data have been obtained for the following biol. relevant lipids: the fatty acids palmitic, stearic, oleic, linoleic, .alpha.-linolenic, and arachidonic acids; the phospholipids 1-stearoyl-2-linoleoyl-3-glycerophosphorylcholine. 1,2-Distearoyl-3-glycerophosphorylcholine, phosphatidylcholine-choline-N-methyl-¹³C, sphingomyelin-choline-N-methyl-¹³C; sphinganine (dihydrosphingosine), 4t-sphingenine (sphingosine), and 3-dehydrosphinganine. Accurate assignments of resonance lines were ascertained using synthetic compds. labeled with .apprx.90% ¹³C in specific positions of the resp. mol. and substituted differentially. The parameters detg. the chem. shifts were analyzed.

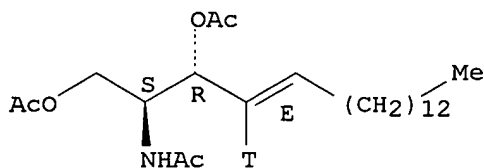
IT 40747-69-1

RL: PRP (Properties)
(NMR of)

RN 40747-69-1 CAPLUS

CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl-3-t]-, [R-[R*,S*-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L32 ANSWER 65 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1972:127356 CAPLUS
 DOCUMENT NUMBER: 76:127356
 TITLE: Molecular arrangements in glycosphingolipids
 AUTHOR(S): Abrahamsson, Sixten; Pascher, Irmin; Larsson, Kare;
 Karlsson, Karl A.
 CORPORATE SOURCE: Swed. Med. Res. Counc. Unit Mol. Struct. Anal., Univ.
 Goteborg, Goteborg, Swed.
 SOURCE: Chem. Phys. Lipids (1972), 8(2), 152-79
 CODEN: CPLIA4
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Homogeneous glycosphingolipids are prepd. and their structural behavior studied in the solid state as well as in lipid-water systems and in surface films. Mainly x-ray diffraction techniques are used in the phase anal. A very complex phase pattern is usually found-e.g., cerebroside contg. 2-hydroxy fatty acids has 5 cryst. phases and 2 thermotropic mesophases. This is also the case in the water systems, where hexagonal, lamellar, and cubic mesophases are obsd. Whereas in earlier surface film studies of complex lipids, such as phospholipids, only one liq. expanded phase usually has been found, cerebroside also exhibit numerous condensed phases. Comparisons with corresponding natural lipids show a close relation both in the phase behavior and structure of the different polymorphs.

IT 2482-37-3

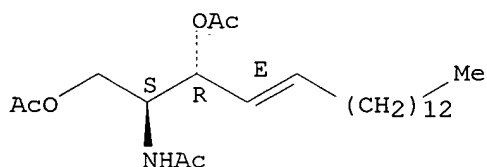
RL: PROC (Process)
 (structural behavior of, in solid liq. and soln. states)

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

Double bond geometry as shown.



L32 ANSWER 66 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1971:485024 CAPLUS
 DOCUMENT NUMBER: 75:85024
 TITLE: Thin-layer chromatography of ceramides
 AUTHOR(S): Karlsson, Karl L.; Pascher, Irmin
 CORPORATE SOURCE: Dep. Med. Biochem., Univ. Goteborg, Goteborg, Swed.
 SOURCE: J. Lipid Res. (1971), 12(4), 466-72
 CODEN: JLPRAW
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Ceramides with mono-, di-, and trihydroxy long-chain bases, and normal (satd. and unsatd.), branched-chain, and 2-hydroxy fatty acids were analyzed by thin-layer chromatog. In most cases the compds. were also run as acetates. Borate, arsenite, and Ag⁺ were used as complexing agents, and the effects of no., position, and stereochemistry of OH groups, and of unsatn., were studied. The results are discussed in view of anal. of natural ceramide species.

IT 2482-37-3 34227-61-7 34249-35-9

34249-37-1 34435-03-5

Searched by Barb O'Bryen & Toby Port

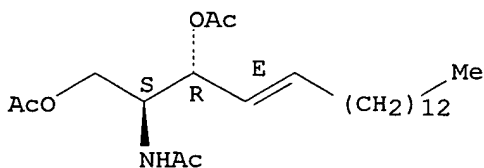
RL: ANT (Analyte); ANST (Analytical study)
(chromatog. of)

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

Double bond geometry as shown.

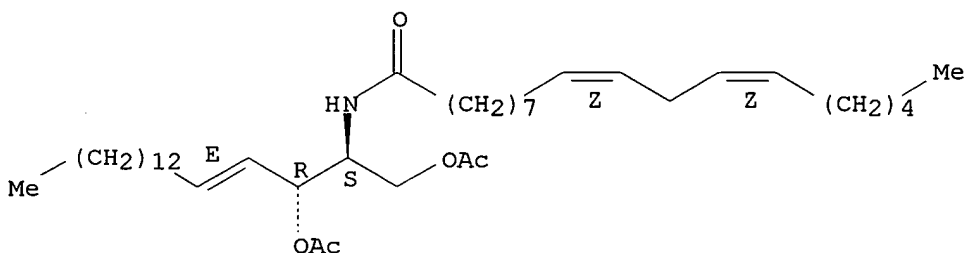


RN 34227-61-7 CAPLUS

CN Linoleamide, N-[2-hydroxy-1-(hydroxymethyl)-3-heptadecenyl]-, diacetate (ester), (E)-D-erythro- (8CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

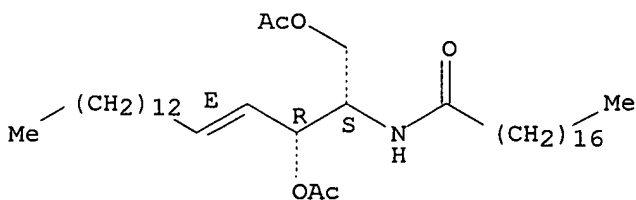


RN 34249-35-9 CAPLUS

CN Octadecanamide, N-[2-hydroxy-1-(hydroxymethyl)-3-heptadecenyl]-, diacetate (ester), (E)-D-erythro- (8CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

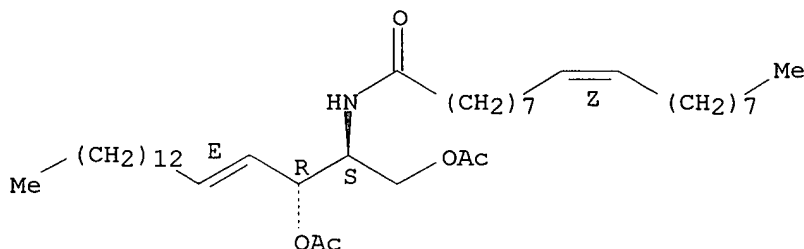


RN 34249-37-1 CAPLUS

CN Oleamide, N-[2-hydroxy-1-(hydroxymethyl)-3-heptadecenyl]-, diacetate (ester), (E)-D-erythro- (8CI) (CA INDEX NAME)

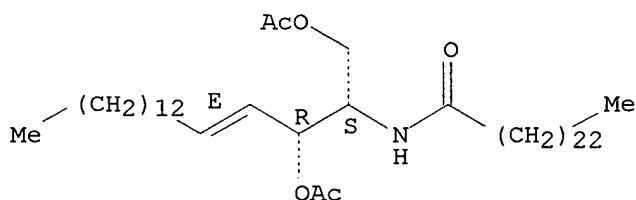
Absolute stereochemistry.

Double bond geometry as shown.



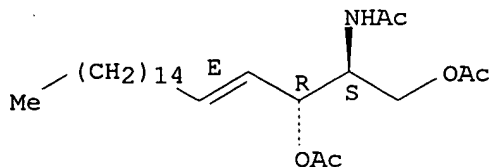
RN 34435-03-5 CAPLUS
 CN Tetracosanamide, N-[2-hydroxy-1-(hydroxymethyl)-3-heptadecenyl]-, diacetate (ester), (E)-D-erythro- (8CI) (CA INDEX NAME)

Absolute stereochemistry.
 Double bond geometry as shown.



L32 ANSWER 67 OF 72 CAPLUS COPYRIGHT 2000 ACS
 ACCESSION NUMBER: 1970:99972 CAPLUS
 DOCUMENT NUMBER: 72:99972
 TITLE: Lipids. Synthesis of C20-sphingosine
 AUTHOR(S): Zvonkova, E. N.; Vlahliiska, T. D.; Soldatova, S. A.; Mitsner, B. I.; Preobrazhenskii, N. A.
 CORPORATE SOURCE: Mosk. Inst. Tonkoi Khim. Tekhnol. im. Lomonosova, Moscow, USSR
 SOURCE: Zh. Org. Khim. (1970), 6(1), 58-62
 CODEN: ZORKAE
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian
 AB Condensation of 2-trans-octadecenyl chloride with AcCHNaCO2Et gave Me(CH2)14CH:CHCOCHAcCO2Et (I). I with PhN2+Cl- in a buffered soln. gave Me(CH2)14CH:-CHCOC(:NNPh)CO2Et which was reduced with Zn/AcOH to Me(CH2)14CH:CHCOCH(NHAc)CO2Et (II). Redn. of II with NaBH4 gave Me(CH2)14CH:CHCH(OH)CH(NHAc)CO2Et (III) (2 isomers sepd. by fractional crystn.). Deacetylation of erythro-III gave Me(CH2)14CH:CHCH(OH)CH(NH2.HCl)CO2Et, which was reduced with LiAlH4 to C20-sphingosine, which was addnl. characterized as Me(CH2)14CH:CHCH(OAc)CH(NHAc)CH2OAc.
 IT **25494-35-3P**
 RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)
 RN 25494-35-3 CAPLUS
 CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-nonadecenyl]-, [R-[R*,S*-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
 Double bond geometry as shown.



L32 ANSWER 68 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1970:48667 CAPLUS

DOCUMENT NUMBER: 72:48667

TITLE: Crystal structure of triacetyl-sphingosine

AUTHOR(S): O'Connell, A. M.; Pascher, I.

CORPORATE SOURCE: Med. Res. Counc. Unit, Univ. Goteborg, Goteborg, Swed.

SOURCE: Acta Crystallogr., Sect. B (1969), 25(Pt. 12), 2553-61

CODEN: ACBCAR

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The crystal structure of triacetyl-sphingosine (D-erythro-1,3-diacetoxy-2-acetamido-4-trans-octadecene, C₂₄H₄₃O₅N) has been detd. by direct methods. The crystals are orthorhombic, P2₁2₁2₁, with a 5.002, b 8.709, and c 60.62 Å. Positional and isotropic thermal parameters of the non-H atoms were refined to give a final R index of 0.109. The mols. are arranged head-to-tail in layers within which the C chains pack according to the common orthorhombic subcell, O .perp.. The chain axis forms an angle of 58.degree. with the end group planes. Adjacent layers show opposite tilt of the chains. In spite of the bulky acetyl branches, the mols. adopt a very effective packing (dm = 1.07). The mols. are connected by a continuous system of N-H-O hydrogen bonds parallel to a, and there is also evidence for 2 weaker C-H-O type interactions.

IT 2482-37-3

RL: PRP (Properties)

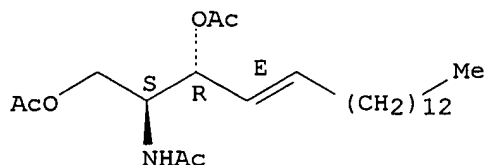
(crystal structure of)

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

Double bond geometry as shown.



L32 ANSWER 69 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1969:509739 CAPLUS

DOCUMENT NUMBER: 71:109739

TITLE: Preparation of ceramides from brain gangliosides and the nature of the sphingosine bases

AUTHOR(S): Klenk, Ernst; Huang, Richard T. C.

CORPORATE SOURCE: Univ. Koeln, Cologne, Ger.

SOURCE: Hoppe-Seyler's Z. Physiol. Chem. (1969), 350(9), 1081-7

CODEN: HSZPAZ

DOCUMENT TYPE: Journal

Searched by Barb O'Bryen & Toby Port

LANGUAGE: German

AB Ganglio-ceramides were prepd. in practically quant. yield from brain gangliosides, following oxidn. with periodate, redn. with NaBH₄, and mild acid hydrolysis. The mixt. of sphingosine bases obtained from them was sepd. into its individual components by the counter-current distribution of the triacetyl compds.; the triacetyl deriv. of C₂₀-sphingosine was isolated for the first time. The yield was 40% of the original mixt. of the sphingosine bases. The properties of the isolated substance agree with the structure D-erythro-1,3-dihydroxy - 2-amino-trans-4-eicosene.

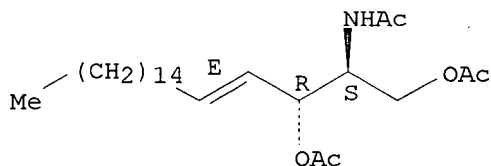
IT 25494-35-3

RL: ANST (Analytical study)
(from gangliosides, of brain)

RN 25494-35-3 CAPLUS

CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-nonadecenyl]-, [R-[R*,S*-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L32 ANSWER 70 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1968:48956 CAPLUS

DOCUMENT NUMBER: 68:48956

TITLE: Metabolism of sphingosine bases. III. Chemical syntheses of carbon-14 and tritium labeled erythro- and threo-dihydrosphingosines and sphingosines

AUTHOR(S): Stoffel, Wilhelm; Sticht, Guido

CORPORATE SOURCE: Univ. Cologne, Cologne, Ger.

SOURCE: Hoppe-Seyler's Z. Physiol. Chem. (1967), 348(12), 1561-9

CODEN: HSZPAZ

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Labeled sphingosines and dihydrosphingosines were prepd. for use in biochem. research. Acrolein was brominated in ether to give 2,3-dibromopropanal, whose di-Et, acetal (I), b₁₃ 108-12.degree., n_{20D} 1.4969, was formed by treatment with HC(OEt)₃ and EtOH. I was dehalogenated with NaNH₂ in liq. NH₃, giving propynal di-Et acetal (II), b₇₆₀ 138-40.degree. and n_{20D} 1.4141. LiC.tplbond.CCH(OEt)₂ was then formed in NH₃ from II and treated with 1-bromotridecane, giving 2-hexadecyne-1-al di-Et acetal (III), b_{0.01125}.degree., n_{20D} 1.4490. III was catalytically reduced in an amt. of 3H, giving palmitaldehyde-2,2,3,3-t₄ di-Et acetal, which by acid hydrolysis with simultaneous complete exchange of .alpha.-protons gave palmitaldehyde-3,3-t₂ (IV), b_{0.125-30}.degree., sp. activity 31.2 .mu.Ci/.mu.mole. Condensing IV with nitroethanol gave .apprx.13-17% threo-2-nitrooctadecan-1,3-diol (V), m. 81-2.5.degree., and a mixt. (A) of threo and erythro-isomers, m. 38.degree.. threo-DL-Dihydrosphingosine-5,5-t₂ (VI), m. 93-5.degree., was prepd. by reducing I with Al amalgam in Et₂O. The triacetyl deriv. of VI m. 66.5.degree.. A was treated with BzH and ZnCl₂, giving erythro-5-nitro-4-pentadecyl-(2,2-t₂)-1,3-dioxane, m. 49.degree., which was reduced with Al amalgam to the 5-amino compd., m. 47-9.degree.. This compd. was acetylated with Ac₂O in pyridine, giving the N-acetyl deriv., m. 131.degree.. Hydrolysis with HCl in dioxane gave erythro-DL-

Searched by Barb O'Bryen & Toby Port

dihydrosphingosine-5,5-t2, m. 83.degree., triacetyl deriv. m. 91-2.degree.. The racemate of VI was sepd. into optical antipodes via the L-glutamate, giving the threo-(+)-L-dihydrosphingosine. The C-acylation of Na acetoacetate by the method of Helferich gave Et 2-acetyl-3-oxooctadecanoate-3-14C, which gave the 2-phenylhydrazone by the Japp-Klingemann reaction. Treatment with Zn in HCO2H gave the 2-amino compd. (VII), m. 122-4.degree.. The LiAlH4 redn. of the 3-oxo group gave the desired erythro- and threo-dihydrosphingosines-3-14C. The diastereomeric mixt. was transformed into the N-dichloroacetyl deriv. and the cryst. erythro form, m. 138.degree., was hydrolyzed to give the free pure erythro compd., m. 83-4.degree.. The LiAlH4 redn. of IV, followed by isomer sepn. as before, gave the erythro-DL-dihydrosphingosine-1,1-t2-3-14C, m. 84.5.degree.. 2-Tetradecyn-1-al di-Et acetal, b0.1 138-45.degree., was prepd. as above, and hydrogenated with 3H to give myristaldehyde-3,3-t2. Condensation with malonic acid gave hexadecanoic-5,5-t2 acid, m. 49.degree., which was converted to the chloride, b0.005 135.degree., n25D 1.4644. Et 2-acetyl-3-oxooctadecenoate-7,7-t2, m. 35.degree., and the phenylhydrazone of Et 2,3-dioxo-4-trans-octadecenoate-7,7-t2, m. 54-6.degree., Et 2-acetamido-3-oxo-4-trans-octadecenoate-7,7-t2, m. 65.degree., Et 2-acetamido-3-hydroxy-4-trans-octadecenoate-7,7-t2, m. 56.degree., and Et 2-amino-3-hydroxyoctadecenoate-7,7-t2 hydrochloride, m. 108-10.degree., were prepd. by previously given methods. The latter compd. was reduced with LiAlH4, giving erythro-DL-sphingosine-7,7-t2, m. 67.degree., triacetyl deriv. m. 89.5.degree..

IT 21300-78-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 21300-78-7 CAPLUS

L32 ANSWER 71 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1967:508121 CAPLUS

DOCUMENT NUMBER: 67:108121

TITLE: Synthesis of DL-erythro and threo-sphingosine-4,5-3H

AUTHOR(S): Gal, Andrew E.

CORPORATE SOURCE: Natl. Inst. of Neurological Diseases and Blindness,
Natl. Inst. of Health, Bethesda, Md., USA

SOURCE: J. Labelled Compd. (1967), 3(2), 112-19

CODEN: JLCAAI

DOCUMENT TYPE: Journal

LANGUAGE: English

AB DL-erythro-Sphingosine (Ia) and DL-threo-sphingosine (II)

[Me(CH2)12CH:CH(OH)CH(NH2)CH2OH] specifically labeled with 3H in positions 4 and 5 were prepd. The synthesis of these compds. was based on a modification of a procedure by Grob and Gadiant (CA 52: 7202h). Quant. sepn. of the sphingosines from acetylenic impurities was accomplished, and the phys. consts. of pure I and II were detd. I was prepd. by resolving the DL racemate and it was identical to the naturally occurring product. 16 references.

IT 2482-37-3P

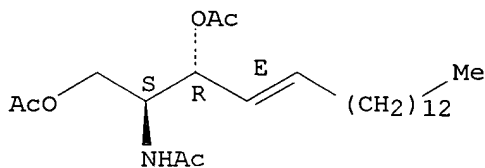
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

Double bond geometry as shown.



L32 ANSWER 72 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1967:481783 CAPLUS

DOCUMENT NUMBER: 67:81783

TITLE: Sphingolipids. II. Synthesis of ceramide-like compounds

AUTHOR(S): Auer, E.; Libert, Hermann; Schmid, Leopold

CORPORATE SOURCE: Univ. Vienne, Vienna, Austria

SOURCE: Monatsh. Chem. (1967), 98(3), 802-6

CODEN: MOCHAP

DOCUMENT TYPE: Journal

LANGUAGE: German

AB cf. CA 67: 2727z. DL-threo-Me(CH₂)₁₂C.tplbond.CCH(OH)CH(NH₂)CH₂OH was hydrogenated using Lindlar catalyst at 20.degree. to give 90% DL-threo-cis-Me(CH₂)₁₂CH:CHCH(OH)CH(NH₂)CH₂OH (I). I gave by further hydrogenation 82% DL-threo-Me(CH₂)₁₄CH(OH)CH(NH₂)CH₂OH, m. 98-100.degree.. I (1 g.) in 20 ml. HCONMe₂ and 0.3 ml. dry pyridine was treated with 1.3 g. lignoceric acid chloride in 15 ml. HCONMe₂ to give DL-threo-cis-Me(CH₂)₁₂CH:CHCHRCH[NHCO(CH₂)₂₂Me]CH₂R' (II) (R = R' = OH) (III), m. 100-2.degree.. Similarly was prepd. DL-threo-cis-Me(CH₂)₁₂CH:CHCHRCH[NHCO(CH₂)₁₂Me]CH₂R' (IV) (R = R' = OH), m. 96.5-98.degree.. III in tetrahydrofuran and pyridine treated with 0.6 g. Ph₃CCl gave 67% II (R = OH, R' = OCPH₃). Similarly was prepd. IV (R = OH, R' = OCPH₃) in 79% yield. II (R = OAc, R' = OCPH₃), II (R = OAc, R' = OH), (m. 95.5-97.degree.), IV (R = OAc, R' = OCPH₃), and IV (R = OAc, R' = OH) (m. 93-5.degree.) were prepd. as usual. II (R = R' = OAc), m. 67-8.degree., was prepd. in 75% yield from III by acetylation.

IT 17673-77-7P

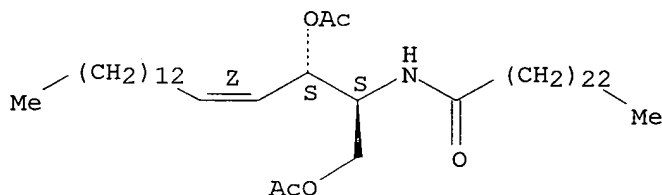
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 17673-77-7 CAPLUS

CN Tetracosanamide, N-[2-hydroxy-1-(hydroxymethyl)-3-heptadecenyl]-, diacetate (ester), (Z)-DL-threo- (8CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.



FILE 'CAOLD' ENTERED AT 16:06:39 ON 07 JUL 2000

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Searched by Barb O'Bryen & Toby Port

FILE COVERS 1907-1966

FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

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=> d que nos 133

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L7          STR
L10         650 SEA FILE=REGISTRY SUB=L4 SSS FUL L7
L28         STR
L31         46 SEA FILE=REGISTRY SUB=L10 SSS FUL L28
L33         13 SEA FILE=CAOLD ABB=ON PLU=ON L31
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L33 ANSWER 1 OF 13 CAOLD COPYRIGHT 2000 ACS

ACCESSION NUMBER: CA65:17257g CAOLD

TITLE: phys. studies of phospholipids - (IV) high resolution nuclear magnetic resonance spectra of phospholipids and related substances

AUTHOR NAME: Chapman, Dennis; Morrison, A.

TITLE: properties of phosphatides prepd. from rice bran and Phaseolus aureus

AUTHOR NAME: Talwalkar, R. T.; Garg, N. K.; Krishna Murti, C. R.

INDEX TERM: 67-48-1 102-76-1 122-32-7 555-43-1 816-93-3
1071-23-4 2462-63-7 **2482-37-3** 3338-29-2
4826-71-5 5683-50-1 5683-54-5 7768-08-3 14479-96-0
14672-00-5 14834-15-2 15557-11-6 16777-83-6
96579-26-9 106065-93-4 106571-73-7

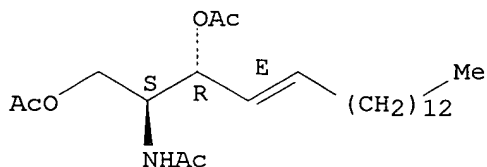
IT **2482-37-3** **96579-26-9**

RN 2482-37-3 CAOLD

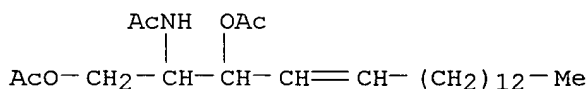
CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

Double bond geometry as shown.



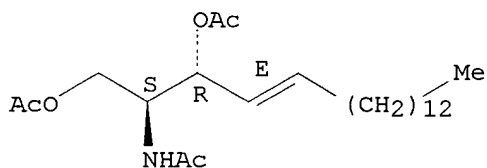
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 (CA INDEX NAME)



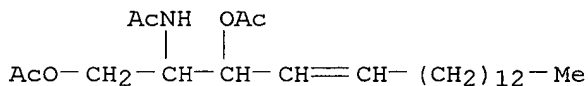
L33 ANSWER 2 OF 13 CAOLD COPYRIGHT 2000 ACS
 ACCESSION NUMBER: CA62:9754e CAOLD
 TITLE: sepn. of long-chain bases by thin-layer chromatography-
 instability of sphingosine
 AUTHOR NAME: Weiss, Benjamin; Stiller, R. L.
 INDEX TERM: 123-78-4 764-22-7 992-35-8 2304-74-7 2304-75-8
 2304-76-9 2304-77-0 2304-78-1 2304-80-5 2304-81-6
 2304-82-7 2458-06-2 **2482-37-3** 2673-72-5
 2675-54-9 2675-55-0 2675-56-1 2675-57-2 2872-63-1
 30684-99-2 38107-88-9 54336-64-0 94381-13-2 94381-57-4
 95423-51-1 **96579-26-9** 96673-02-8 96772-09-7
 96772-16-6

IT **2482-37-3 96579-26-9**
 RN 2482-37-3 CAOLD
 CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).
 Double bond geometry as shown.



RN 96579-26-9 CAOLD
 CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI)
 (CA INDEX NAME)



L33 ANSWER 3 OF 13 CAOLD COPYRIGHT 2000 ACS
 ACCESSION NUMBER: CA62:6843a CAOLD
 TITLE: structural components of the pyridine-insol. sphingolipid
 Searched by Barb O'Bryen & Toby Port

from *Corbicula sandai*, and the distribution in other species

AUTHOR NAME: Hori, Taro; Itasaka, O.; Inoue, H.; Yamada, K.
 INDEX TERM: 501-11-1 2041-14-7 2461-23-6 **2482-37-3**
 7518-10-7 **96579-26-9**

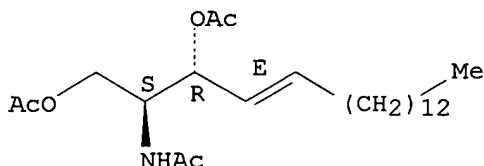
IT **2482-37-3 96579-26-9**

RN 2482-37-3 CAOLD

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

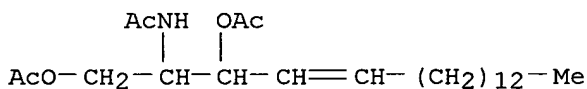
Absolute stereochemistry. Rotation (-).

Double bond geometry as shown.



RN 96579-26-9 CAOLD

CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI)
 (CA INDEX NAME)



L33 ANSWER 4 OF 13 CAOLD COPYRIGHT 2000 ACS

ACCESSION NUMBER: CA58:12407b CAOLD

TITLE: action of esters of chlorosulfurous acid on alkyl
 sulfates-prepn. of diethyl sulfate

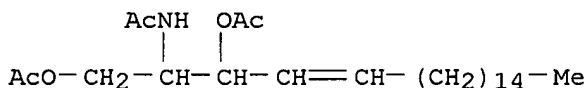
AUTHOR NAME: Kraft, M. Ya.; Lyutina, F. V.

INDEX TERM: 24028-07-7 **96770-39-7**

IT **96770-39-7**

RN 96770-39-7 CAOLD

CN Acetamide, N-[2-hydroxy-1-(hydroxymethyl)-3-nonadecenyl]-, diacetate (7CI)
 (CA INDEX NAME)



L33 ANSWER 5 OF 13 CAOLD COPYRIGHT 2000 ACS

ACCESSION NUMBER: CA58:11370g CAOLD

TITLE: sphingosine, stereospecific syntheses of compds. related to

PATENT ASSIGNEE: CIBA Ltd.

DOCUMENT TYPE: Patent

PATENT NO.	KIND	DATE
GB 864261		

PI GB 864261

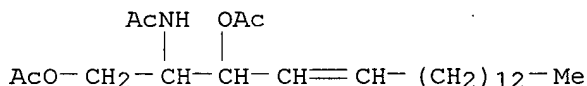
INDEX TERM: 13552-54-0 94375-81-2 94676-99-0 95220-02-3
96579-26-9 97258-24-7 97282-27-4 97282-28-5
 101635-19-2

IT **96579-26-9**

RN 96579-26-9 CAOLD

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CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI)
(CA INDEX NAME)



L33 ANSWER 6 OF 13 CAOLD COPYRIGHT 2000 ACS

ACCESSION NUMBER: CA55:23611f CAOLD

TITLE: effect of mevalonate analogs on cholesterol biosynthesis

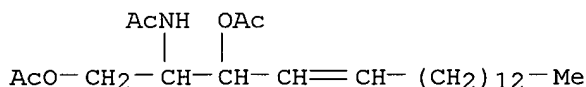
AUTHOR NAME: Weiss, Herbert; Schiffman, E.; Titus, E. O.

INDEX TERM: 13552-09-5 96579-26-9

IT 96579-26-9

RN 96579-26-9 CAOLD

CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI)
(CA INDEX NAME)



L33 ANSWER 7 OF 13 CAOLD COPYRIGHT 2000 ACS

ACCESSION NUMBER: CA55:19796c CAOLD

TITLE: 2,2,4,6,6-pentachloro-5-oxo-3-hexenoic acid esters

PATENT ASSIGNEE: Ruhrchemie Akt.-Ges.

DOCUMENT TYPE: Patent

TITLE: esters of 2,2,4,6,6-pentachloro-5-oxo-3-hexenoic acid

AUTHOR NAME: Feichtinger, Hans; Puschhof, S.

DOCUMENT TYPE: Patent

PATENT NO.	KIND	DATE
DE 1056119		

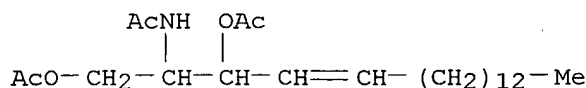
PI DE 1056119

INDEX TERM: 13552-54-0 96579-26-9 108128-78-5 108128-79-6
114379-89-4 117882-92-5

IT 96579-26-9

RN 96579-26-9 CAOLD

CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI)
(CA INDEX NAME)



L33 ANSWER 8 OF 13 CAOLD COPYRIGHT 2000 ACS

ACCESSION NUMBER: CA55:19795e CAOLD

TITLE: 1,3-dihydroxy-2-amino-4-alkenes, stereospecific method for
the prepn. of

PATENT ASSIGNEE: CIBA Ltd.

DOCUMENT TYPE: Patent

TITLE: prepn. of 1,3-dihydroxy-2-amino-4-alkenes

AUTHOR NAME: Grob, Cyril A.

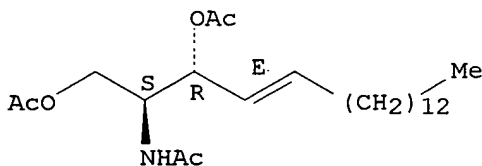
DOCUMENT TYPE: Patent

PATENT NO.	KIND	DATE

Searched by Barb O'Bryen & Toby Port

$$\text{AcO}-\text{CH}_2-\overset{\text{AcNH}}{\underset{|}{\text{CH}}}-\overset{\text{OAc}}{\underset{|}{\text{CH}}}-\text{CH}=\text{CH}-(\text{CH}_2)_{12}-\text{Me}$$

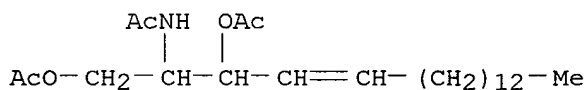
Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.


$$\text{AcO}-\text{CH}_2-\overset{\text{AcNH}}{\underset{|}{\text{CH}}}-\overset{\text{OAc}}{\underset{|}{\text{CH}}}-\text{CH}=\text{CH}-(\text{CH}_2)_{12}-\text{Me}$$

L33 ANSWER 11 OF 13 CAOLD COPYRIGHT 2000 ACS
ACCESSION NUMBER: CA52:7202h CAOLD
Searched by Barb O'Bryen & Toby Port

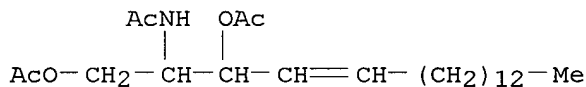
TITLE: synthesis of sphingosine and its stereoisomers
 AUTHOR NAME: Grob, Cyril A.; Gadiant, F.
 INDEX TERM: 765-09-3 765-13-9 13552-12-0 13552-54-0 18696-97-4
 51534-40-8 94375-81-2 94676-99-0 95220-02-3
 96579-26-9 101635-19-2 114697-01-7 115097-86-4

IT 96579-26-9
 RN 96579-26-9 CAOLD
 CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI)
 (CA INDEX NAME)



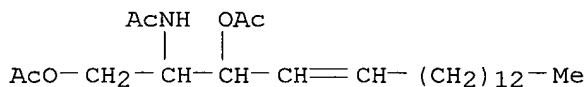
L33 ANSWER 12 OF 13 CAOLD COPYRIGHT 2000 ACS
 ACCESSION NUMBER: CA51:4272c CAOLD
 TITLE: sphingolipide series - (IV) detn. of the configuration of
 the amino C atom in sphingosine
 AUTHOR NAME: Prostenik, M.; Munk-Weinert, M.; Sunko, D. E.
 INDEX TERM: 13552-54-0 16538-04-8 26547-18-2 96579-26-9
 103043-32-9 103043-93-2 103044-19-5 103044-86-6 103045-14-3
 103047-85-4 122389-37-1

IT 96579-26-9
 RN 96579-26-9 CAOLD
 CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI)
 (CA INDEX NAME)



L33 ANSWER 13 OF 13 CAOLD COPYRIGHT 2000 ACS
 ACCESSION NUMBER: CA51:1035h CAOLD
 TITLE: cyclic sulfites derived from the chloropropanediols
 AUTHOR NAME: De la Mare, P. B. D.; Klyne, W.; Millen, D. J.; Pritchard,
 J. G.; Watson, D.
 INDEX TERM: 96-24-2 497-04-1 1469-73-4 3741-38-6 4176-55-0
 4176-57-2 15121-11-6 96579-26-9 122330-92-1

IT 96579-26-9
 RN 96579-26-9 CAOLD
 CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI)
 (CA INDEX NAME)



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